Application Note
31109

Mini-disk 525

An Efficient Approach to Extract over **100 Semi-Volatile Organic** Compounds using **SPE Mini-disks** with **Automated SPE Systems**

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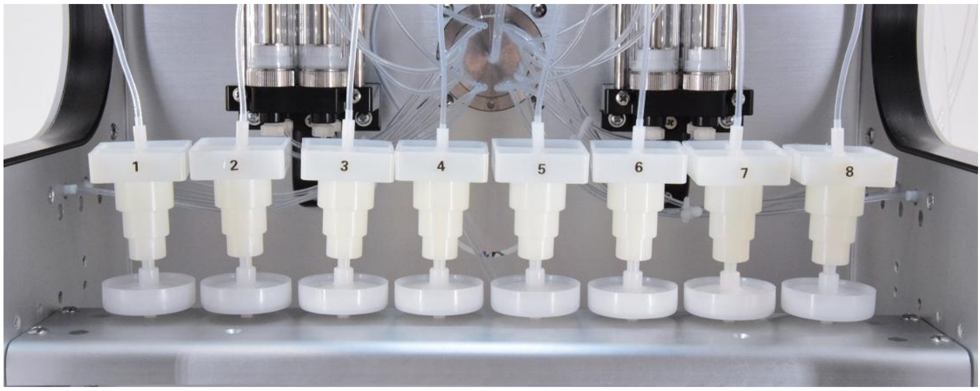


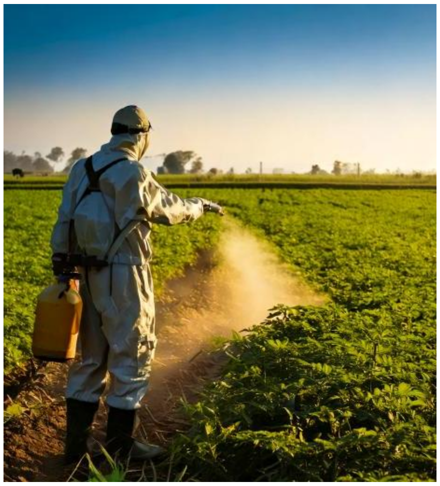
Keywords

EPA Method 525, semi-volatiles, pesticides, PAHs, PCBs, phthalates, Mini-disk, SPE-03, Presto Automated SPE, water

ABSTRACT

Solid phase extraction (SPE) is commonly used in the analysis of semi-volatile organic compounds (SVOCs) in drinking water. To capture the full advantages of SPE disks and cartridges, PromoChrom developed a suite of Mini-disks which come in a format similar to a 30 mm syringe filter and have a cross-sectional area 5 times that of a 6 mL SPE cartridge. The increased cross-sectional area and optimized sorbent properties enable the Mini-disks to work with much higher flow rates than SPE cartridges while consuming less solvent than SPE disks. Its compact size makes it easily adaptable to any PromoChrom automated extraction system, especially when paired with the latest Presto automated SPE system, which significantly shortens the time needed for sample loading. This application note demonstrates the extraction of over 100 SVOCs (plus surrogates) in water using our MD-525-30 Mini-disk with both the SPE-03 and Presto automated SPE systems verified in-house at PromoChrom.

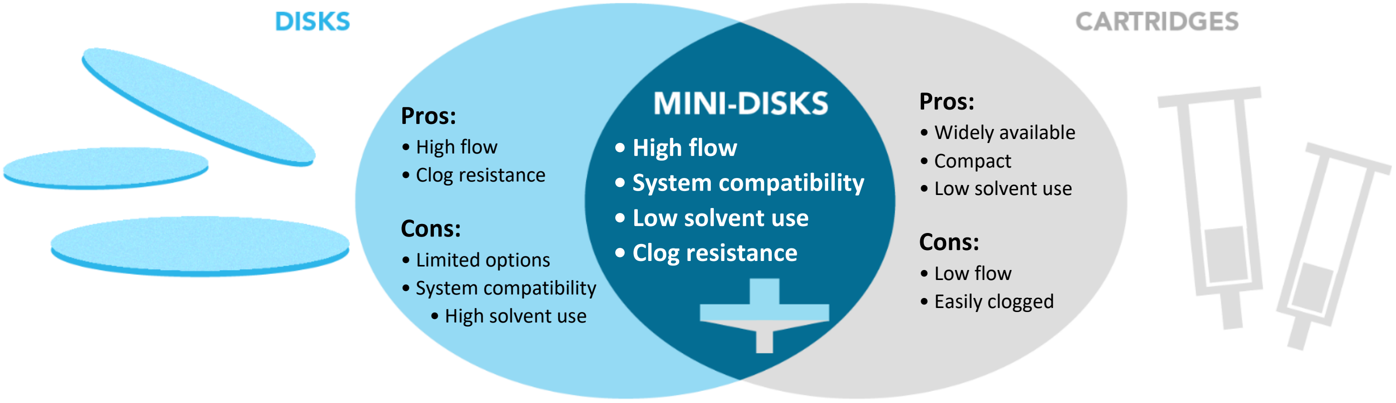
INTRODUCTION



Due to industrial activities, agricultural runoff, and urban pollution, contamination of common drinking water has become a major concern. Among the substances under scrutiny, the most common are pesticides, polychlorinated biphenyls (PCBs), Polycyclic Aromatic Hydrocarbons (PAHs) and phthalate residues. Detecting and measuring trace levels of these compounds in water is crucial for ensuring compliance with environmental regulations and protecting drinking water supplies.

EPA method 525.3 is a method for the determination of SVOCs in drinking water by solid phase extraction (SPE) and capillary column Gas Chromatography-Mass Spectrometry (GCMS). On top of EPA Method 525.2, version 525.3 introduces some improvements such as using matrix-matched standards, spiking internal standard just before analysis on GCMS and removing some problematic compounds from the target list. Per these methods, 1 L sample is extracted with LSE cartridges, SPE disks, or SPE cartridges. Even though SPE disks offer faster sample loading speed and better tolerance to clogging, they require more solvent usage and have limited market options and compatibility with automated systems. SPE cartridges are more affordable, widely available and compatible with most extraction platforms.

In this application note, we bring forth a novel Mini-disk that combines the advantages and addresses the shortcomings of cartridges and disks. The diameter of the Mini-disk measures only 30 mm and is packaged to fit standard luer slip connections, making it suitable for cartridge-based automated SPE systems and vacuum manifolds. In combination with both the PromoChrom SPE-03 and Presto automated SPE systems, a 50 mL/min flow rate can be achieved for the conditioning and sample loading processes. The total extraction time is 137 minutes for the SPE-03 and 79 minutes for the Presto with total collection solvent volume being less than 20 mL for both systems.



This application note demonstrates a series of in-house tests using MD-525-30 Mini-disk with the SPE-03 and Presto systems to extract over 100 SVOCs from water samples for analysis.

MATERIALS

- Standards for sample spiking and GCMS analysis:

  PCB Congener mix for 525.2 (Restek, part number 32420); Method 525.2 Nitrogen/Phosphorous Pesticide Mix (Restek, part number 32423); Organophosphorus Pesticide Mix (Restek, part number 33013); OrganoNitrogen Pesticide Mix for 525.2 (Restek, part number 33012); Organochlorine Pesticide Mix#1 (Restek, 32415); Method 525.2 Semivolatile Mix (Restek, 31899); Organochlorine Pesticide Mix #2 (Restek 33011).

- Internal standards: Method 525.2 Internal Standard Mix (Restek, 31825), including Acenaphthene-d10, Chrysene-d12 and Phenanthrene-d10.
- Surrogate standards: Method 525.2 Internal Standard Mix (Restek, 31826), including 1,3-Dimethyl-2-nitrobenzene, Perylene-d12, Pyrene-d10 and Triphenylphosphate.
- Mini-disk: PromoChrom Mini-disk packed with mixed-mode polymers capable of extracting both hydrophilic and hydrophobic organic compounds in water (PromoChrom, part number MD-525-30).
- Instrument for Extraction: SPE-03 and Presto 8-channel SPE systems for automatic rinsing of up to 1L sample bottles.
- Instrument for analysis: Agilent GCMS system including a 7890A plus GC with split/splitless inlet, a 7693A autosampler and a 5977B Inert MSD. The column is an Agilent J&W HP-5MS 30 m x 0.25 mm x 0.25 um.

METHODS

Sample Extraction

8 x 1L water samples in 1-liter amber glass bottle were prepared for each of SPE-03 and Presto, 4 following EPA Method 525.2 and 4 following 525.3. For samples following EPA Method 525.2, 0.1g of ascorbic acid was added as preservative and the samples were acidified to pH <2 using 2.0 mL hydrochloric acid (6N). For samples following EPA Method 525.3, 0.1 g of ascorbic acid, 0.35 g of EDTA disodium salt and 9.4 g of potassium dihydrogen citrate were added as preservatives and without further pH adjustment (pH ~3.8). The surrogate and target standards were diluted with ethyl acetate to 50 ug/mL. An aliquot of 40 μL of this stock standard solution (containing 2 μg for each analyte) was mixed with 2 mL methanol and then added to the water samples and mixed well. The internal standards were diluted to 200 ug/mL using ethyl acetate to be added after the extraction and evaporation steps. Samples were extracted using the method shown below. Steps specific to the SPE-03 and Presto are shown in blue and green respectively.

SPE procedures programmed on the SPE-03/Presto
***Solvent 1** = Methanol (MeOH) , **Solvent 2** = Water, **Solvent 3** = Ethyl acetate (EtOAc) , **Solvent 4** = Methylene chloride (DCM),*
***Solvent 5** = DCM:EtOAc (1:1), **Solvent 6** = pH2 water made with HCl; **W1** = Aqueous waste, **W2** = Organic waste*

Action	Inlet 1	Flow	Volume	*Description*
Elute W2	Solvent 4	50 mL/min	5 mL	*Condition Mini-disks with 5 mL of DCM*
Elute W2	Solvent 3	50 mL/min	10 mL	*Condition Mini-disks with 10 mL of EtOAc*
Wait	Time based		1 min	*Allow 1 minute soak*
Elute W2	Solvent 3	50 mL/min	5 mL	*Condition Mini-disks with 5 mL of EtOAc*
Air-Purge W2	Air	50 mL/min	15 mL	*Purge residual solvent from Mini-disks to waste 2*
Elute W2	Solvent 1	50 mL/min	10 mL	*Condition Mini-disks with 10 mL MeOH*

Elute W1	Solvent 6	50 mL/min	10 mL	*Condition Mini-disks with 10 mL pH2 water*
Add Samp W1	Sample	50 mL/min	1050 mL	*SPE03: Load samples at 50 mL/min, using 1050 mL to ensure all sample liquid in the bottles are loaded*
Add Samp W1	Sample	50 mL/min	3 mL	*Presto: Load just 3mL to prime the Presto pumps*
Add Samp+ W1	Sample	50 mL/min	1050 mL	*Presto: Load samples at 50 mL/min through presto pumps, using 1050 mL to ensure all sample liquid in the bottles are loaded*
Elute W1	Solvent 2	50 mL/min	40 mL	*Wash Mini-disks with 40 mL water*
Air-Purge W2	Air	50 mL/min	15 mL	*Remove water droplets from the Mini-disks*
Blow N2	Time based		20 min	*Use nitrogen to dry the disks*
Rinse	Solvent 3	70 mL/min	5 mL	*Rinse sample bottles with 5 mL EtOAc*
Air-Purge R	Air	70 mL/min	5 mL	*Purge rinse lines*
Collect 1	Sample	5 mL/min	10 mL	*Collect rinsate into Fraction 1 through Mini-disks*
Rinse	Solvent 4	70 mL/min	5 mL	*Rinse sample bottles with 5 mL DCM*
Air-Purge R	Air	70 mL/min	5 mL	*Purge rinse lines*
Collect 1	Sample	5 mL/min	10 mL	*Collect rinsate into Fraction 1 through Mini-disks*
Rinse	Solvent 5	70 mL/min	5 mL	*Rinse the sample botter with DCM:EtOAc (1:1)*
Air-Purge R	Air	70 mL/min	5 mL	*Purge rinse lines*
Collect 1	Sample	5 mL/min	15 mL	*Collect rinsate into fraction 1 through Mini-disks*
Collect 1	Solvent 5	5 mL/min	2 mL	*Elute the Mini-disks directly with DCM:EtOAc (1:1) and collect into fraction 1*
Air-Purge 1	Air	5 mL/min	15 mL	*Push any remaining liquid into fraction 1*

The extraction took 137 minutes for a batch of 8 samples using SPE-03 and 79 minutes using Presto. After the "Blow N2" step, an inline drying column containing approximately 16 g of sodium sulfate was attached after each Mini-disk as shown on the right to dry the final extracts as they were eluted. The collected fractions, roughly 13mL, were transferred to 50 mL K-D tubes. After the transfer, 2 mL of DCM was added to the fraction collection tube, vortexed, and poured into the K-D tube. This is repeated with another 1 mL of DCM. The extracts in the K-D tubes are evaporated to <1 mL (above 0.5 mL end point) using a nitrogen evaporator at 38 °C with a N2 flow rate of 0.1-2.3 L/min. The nitrogen flow rate started low at 0.1 – 0.7 L/min to avoid splashing. After evaporation, 25 µL of 200 ppm IS was added, and the volume was adjusted to 1.0 mL with ethyl acetate prior to GC-MS analysis.

SPE-03 with Mini-disks and inline drying columns

Note: Other options for elution solvents include a mixture of EtOAc and DCM, EtOAc alone or a mixture of EtOAc and hexane.

GCMS Analysis

The parameters for GCMS analysis are listed in below:

Parameters for GCMS analysis

Injection Volume	1 µL
Inlet	265 °C; Pulsed splitless injection mode
Oven Temperature Program	50 °C (hold for 1 minutes), 23 °C/min to 150 °C 4 °C/min to 210 °C (hold for 1 minutes) 10 °C/min to 312 °C (hold for 3 minutes) Total run time 35.548 mins
Carrier Gas and Flow Rate	Helium at 1.5 mL/min, constant flow
Transfer Line Temperature	280 °C
Ion Source Temperature	280 °C
Quadrupole Temperature	150 °C
Scan and SIM	45 to 450 *m/z*

RESULTS AND DISCUSSION

The recoveries of **25 commonly analyzed SVOCs** are summarized in Figure 1 and Appendix Table 3. They were all within the EPA Method 525.3 acceptance limits of 70%-130% (60%-130% for HCCP and HCB).

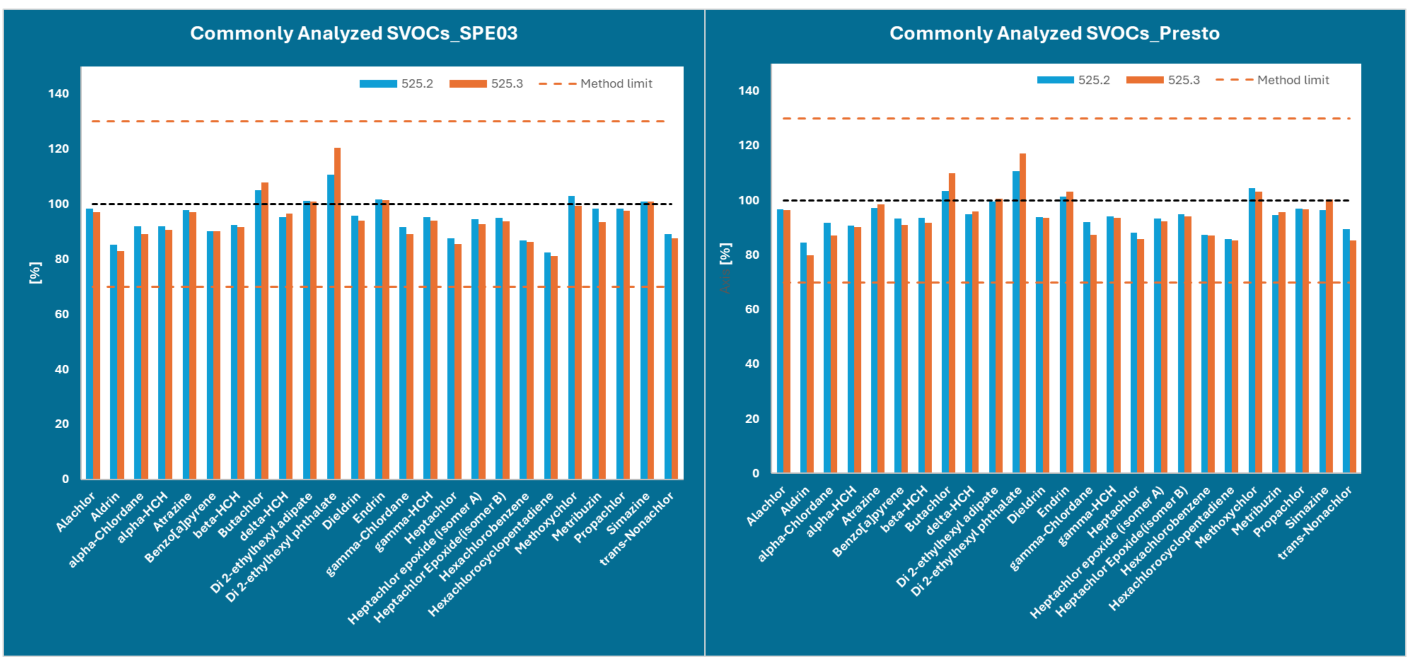


Figure 1 : Commonly analyzed SVOCs recoveries on the SPE-03 and Presto- systems; method limits are illustrated as the orange dashed lines; black dashed line is at 100%.

The recoveries of **17 PAHs** (including one surrogate) on the SPE-03 and Presto systems are summarized in Figure 2 and Appendix Table 4. All analytes were spiked at 2 ppb and all recoveries fall within the 70%-130% range.

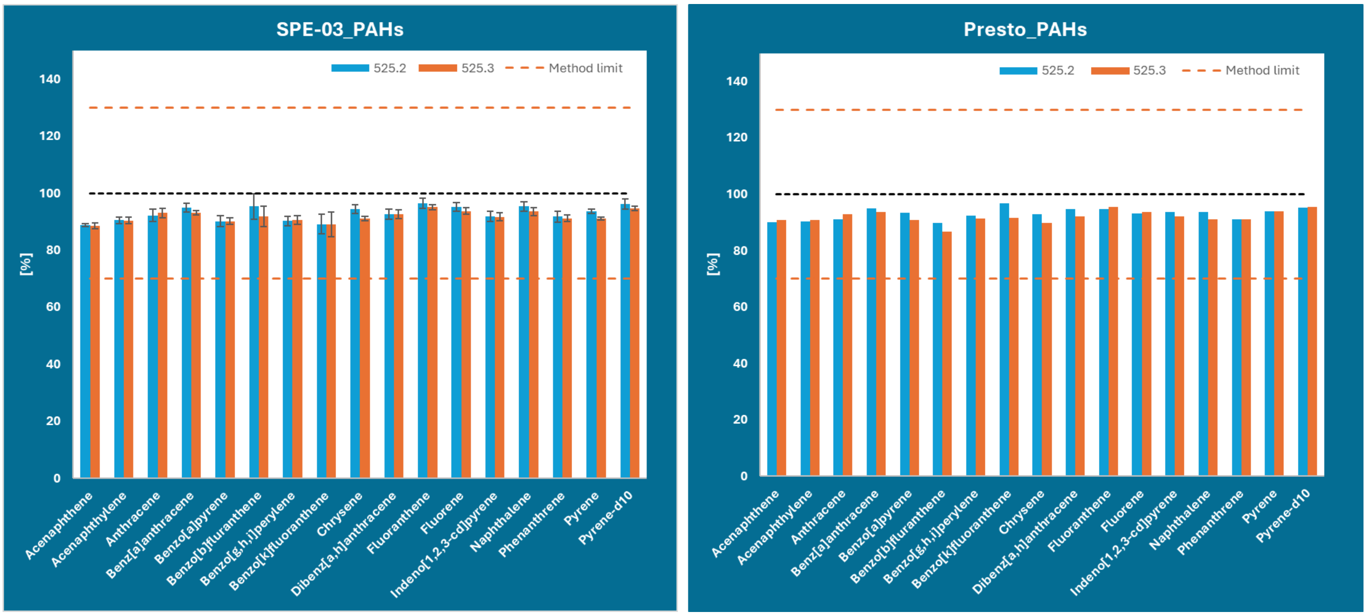


Figure 2: PAHs recoveries on the SPE-03 and Presto systems; method limits are illustrated as the orange dashed lines; black dashed line is at 100%.

The recoveries of **9 PCBs** on SPE-03 and Presto systems are summarized in Figure 3 and Appendix Table 5. All analytes were spiked at 1 ppb and all recoveries fall within the 70%-130% range.

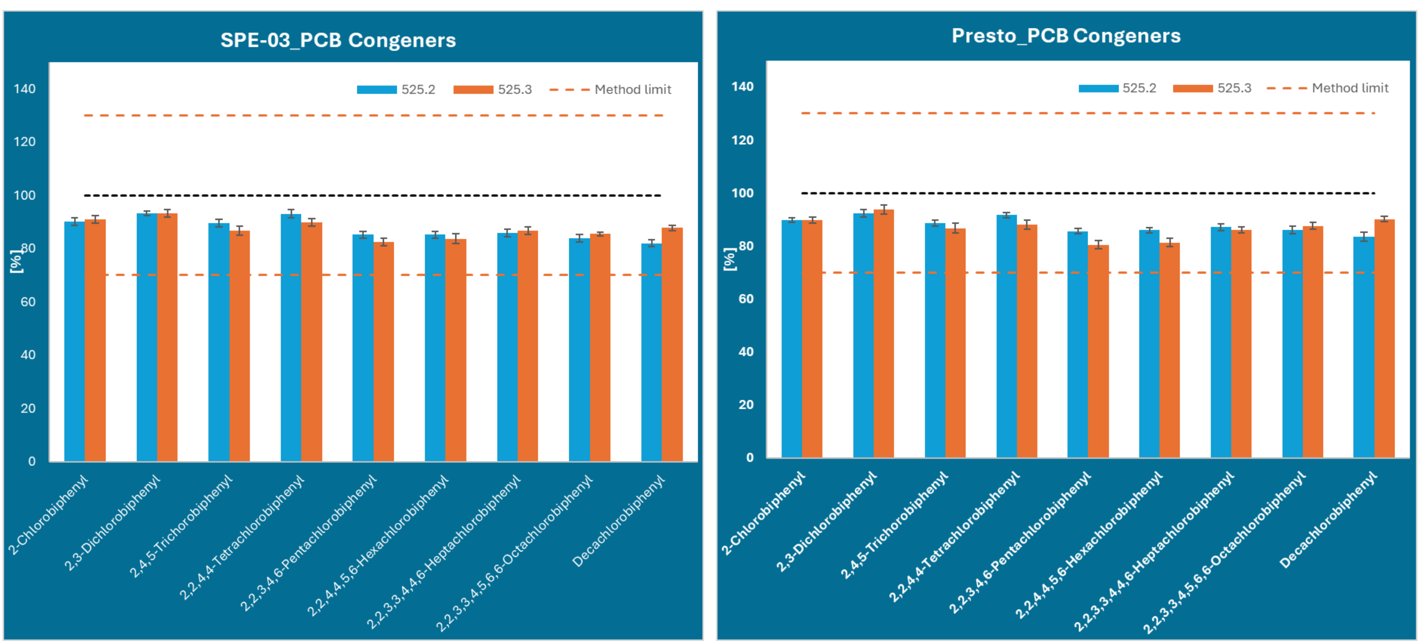


Figure 3 : PCBs recoveries on the SPE-03 and Presto systems; method limits are illustrated as the orange dashed lines; black dashed line is at 100%.

The recoveries of **64 other SVOCs** (and 3 surrogate standard compounds) are summarized in Figure 4 and Appendix Table 6. All analytes were spiked at 2 ppb, and most recoveries fall within the 70-130% range, which meets the criteria of EPA Method 525 (as shown in Figure 4). From the results, Diazinon and Fenamiphos exhibited noticeably different recoveries between methods 525.2 and 525.3. Diazinon undergoes fast hydrolysis in more acidic conditions which resulted in low recoveries at pH < 2 (525.2) and improved recoveries at pH 3.8 (525.3), Fenamiphos had a slight over-recovery with the 525.3 method but near 100% recovery with 525.2, but the exact reasoning is unknown.

Figure 4 : Other SVOCs recoveries on the SPE-03 and Presto-SPE systems; method limits are illustrated as the orange dashed lines; black dashed line is at 100%.

Not included in the results are some compounds that are less compatible with these methods (shown in Appendix Table 2). Carboxin and Methyl Paraoxon, which are also excluded from EPA Method 525.3, exhibited poor chromatographic results at low concentrations and are unstable in water. Disulfoton was also found to be unstable in water and began to degrade almost immediately as mentioned in EPA Method 525.2. Merphos is partially converted to Tribufos (DEF) in aqueous matrices, and when introduced into a hot gas chromatographic injection system. The efficiency of this conversion appears to be unpredictable and not reproducible. Therefore, Merphos cannot be quantified and can only be identified by the presence of DEF in the sample.

Results here are based on PromoChrom's in-house best practices. Laboratories are responsible for meeting the quality control and calibration requirements when following EPA Methods.

CONCLUSION

The PromoChrom MD-525-30 mini-disk in combination with either the SPE-03 or Presto systems can effectively extract over 100 SVOCs (plus 4 surrogates) while meeting the EPA Method 525 recovery and precision criteria. This solution offers an efficient extraction approach taking 137 minutes on the SPE-03 and 79 minutes on the Presto for 8 x 1 L water samples. The controlled extraction time using positive-pressure pumps further provides laboratories with predictable turnaround times. By using only 15 mL of combined DCM and EtOAc for fraction collection and 3 mL of DCM for transferring extracts, this approach aligns well with the EPA's initiative to reduce harmful DCM exposure.

ORDERING INFORMATION FOR MINI-DISKS

Part number	Description	Application
MD-525-30	Packed with 25-um spherical mixed-mode sorbent. 40 Mini-disks per box.	For extraction of hydrophobic and hydrophilic compounds.

REFERENCES

1. EPA method 525.2, EPA Method 525.2: Determination of Organic Compounds in Drinking Water by Liquid-Solid Extractions and Capillary Colum Gas Chromatography/Mass Spectrometry .

2. EPA method 525.3, EPA Method 525.3 - Determination of Semivolatile Organic Chemicals in Drinking Water by Solid Phase Extraction and Capillary Column Gas Chromatography/Mass Spectrometry (GC/MS) | Science Inventory | US EPA

Appendix

Table 1. Internal standards and Surrogates

Internal Standard Compounds

Analyte	CAS #
Acenaphthene-d10	15067-26-2
Chrysene-d12	1719-03-5
Phenanthrene-d10	1517-22-2

Surrogate Standards

Analyte	CAS #
1,3-Dimethyl-2-nitrobenzene	81-20-9
Perylene-d12	1520-96-3
Pyrene-d10	1718-52-1
Triphenylphosphate	115-86-6

Table 2. Problematic compounds

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Carboxin	5234-68-4	26.88	37.51	54.4	9.82	36.16	22.43	49.83	12.86
Diazinon	333-41-5	70.49	4.59	94.44	3.76	78.11	5.52	94.67	2.72
Disulfoton	298-04-4	37.02	39.03	60.94	8.7	39.51	22.18	48.58	12.13
Disulfoton sulfone	2497-06-5	111.41	4.22	113.28	3.32	108.72	1.58	115	2.98
Endrin aldehyde	7421-93-4	101.23	3.95	89.39	5.33	101.22	1.7	97.43	3.31
Endrin ketone	53494-70-5	100.44	4.37	100.79	4.61	102.29	8.27	97.66	4.88
Fenamiphos	22224-92-6	104.56	13.83	140.95	2.64	106.82	9.1	145.65	4.83
Fluridone	59756-60-4	136.33	2.93	136.46	3.05	135.39	2.62	138.5	3.87
Merphos	150-50-5	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Methyl paraoxon	950-35-6	94.52	4.63	98.15	1.88	95.45	4.44	99.61	3.7
Terbufos	13071-79-9	77.12	9.31	85.67	1.77	77.51	4.47	79.64	3.73
Tricyclazole	41814-78-2	117.93	4.57	122.39	4.15	116.24	2.03	125.83	6.79

Note:

1. Merphos is partially converted to DEF in aqueous matrices, and when introduced into a hot gas chromatographic injection system. The efficiency of this conversion appears to be unpredictable and not reproducible. Therefore, Merphos cannot be quantified and can only be identified by the presence of DEF in the sample[1]

2. Carboxin, Disulfoton, and Disulfoton Sulfoxide were found to be unstable in water and began to degrade almost immediately. These analytes may be identified by this method but not accurately measured[1].

3. Most of them are the compounds taken off the list in EPA method 525.3[2].

4. These compounds exhibited poor chromatographic results.

Table 3. Commonly Analyzed SVOCs

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Alachlor	15972-60-8	98.37	3.32	97.09	2.47	96.77	1.51	96.30	2.14
Aldrin	309-00-2	85.26	3.74	82.79	3.08	84.57	1.98	79.82	4.45
alpha-Chlordane	5103-71-9	91.89	2.49	89.15	2.05	91.87	1.90	87.20	2.98
alpha-HCH	319-84-6	91.77	2.87	90.73	2.12	90.60	1.66	90.14	2.51
Atrazine	1912-24-9	97.74	2.23	96.97	1.68	97.07	2.81	98.38	3.08
Benzo[a]pyrene	50-32-8	90.09	3.89	90.16	2.48	93.33	1.74	90.92	3.02
beta-HCH	319-85-7	92.36	2.42	91.67	2.53	93.66	2.26	91.71	2.85
Butachlor	23184-66-9	105.01	3.56	107.76	2.64	103.53	1.48	109.92	2.04
delta-HCH	319-86-8	95.11	2.98	96.58	2.72	94.82	1.78	96.01	2.98
Di 2-ethylhexyl adipate	103-23-1	101.12	3.83	100.94	3.15	99.61	2.58	100.65	3.03
Di 2-ethylhexyl phthalate	117-81-7	110.76	5.46	120.49	4.55	110.67	3.98	117.23	4.21
Diazinon	333-41-5	70.49	4.59	94.44	3.76	78.11	5.52	94.67	2.72
Dieldrin	60-57-1	95.68	3.89	93.92	3.15	93.93	1.77	93.67	2.56
Endrin	72-20-8	101.62	3.72	101.48	1.95	101.44	1.46	103.23	2.76
Fenamiphos	22224-92-6	104.56	13.83	140.95	2.64	106.82	9.1	145.65	4.83
gamma-Chlordane	5103-74-2	91.68	2.84	89.03	2.14	91.97	2.00	87.26	3.20
gamma-HCH	58-89-9	95.10	2.21	93.90	2.23	94.00	1.65	93.67	2.58
Heptachlor	76-44-8	87.52	3.72	85.45	1.85	88.19	1.65	85.79	2.69
Heptachlor epoxide (isomer A)	28044-83-9	94.58	2.97	92.63	1.79	93.35	1.77	92.17	2.70
Heptachlor Epoxide(isomer B)	1024-57-3	94.85	2.78	93.56	2.07	94.86	1.51	93.96	2.62
Hexachlorobenzene	118-74-1	86.78	2.03	86.12	2.77	87.37	1.08	87.13	2.59
Hexachlorocyclopentadiene	77-47-4	82.51	5.87	81.12	3.26	85.74	1.39	85.36	2.55
Methoxychlor	72-43-5	102.83	2.80	99.39	2.98	104.52	1.88	103.10	2.16
Metribuzin	21087-64-9	98.31	3.35	93.51	2.74	94.67	2.69	95.62	3.08
Propachlor	1918-16-7	98.23	1.78	97.49	2.30	96.94	1.61	96.56	2.14
Simazine	122-34-9	100.78	2.79	100.85	2.62	96.52	2.31	100.26	2.37
trans-Nonachlor	39765-80-5	88.95	2.68	87.52	2.23	89.35	1.93	85.29	3.08

Table 4. PAHs

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Acenaphthene	83-32-9	88.89	1.04	88.57	2.08	89.99	1.96	90.78	1.40
Acenaphthylene	208-96-8	90.51	2.26	90.42	2.16	90.42	2.09	90.72	2.82
Anthracene	120-12-7	92.21	4.30	93.02	3.22	90.98	2.81	92.97	3.16
Benz[a]anthracene	56-55-3	94.93	3.16	93.14	1.62	94.95	1.66	93.72	2.83
Benzo[a]pyrene	50-32-8	90.09	3.89	90.16	2.48	93.33	1.74	90.92	3.02
Benzo[b]fluranthene	205-99-2	95.34	8.93	91.86	7.22	89.72	3.71	86.67	4.31
Benzo[g,h,i]perylene	191-24-2	90.19	3.25	90.55	2.91	92.26	1.90	91.29	2.92
Benzo[k]fluoranthene	207-08-9	89.15	6.89	89.08	8.67	96.77	5.21	91.63	4.25
Chrysene	218-01-9	94.30	3.11	91.09	1.62	92.97	3.35	89.73	3.40
Dibenz[a,h]anthracene	53-70-3	92.59	3.41	92.60	2.86	94.61	2.52	92.03	3.81

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Fluoranthene	206-44-0	96.36	3.56	95.09	1.64	94.77	1.88	95.50	1.91
Fluorene	86-73-7	95.10	3.04	93.76	2.08	93.05	2.57	93.76	2.66
Indeno[1,2,3-cd] pyrene	193-39-5	91.77	3.54	91.63	2.77	93.79	1.99	91.99	3.06
Naphthalene	91-20-3	95.31	3.49	93.59	2.78	93.54	1.78	91.02	2.54
Phenanthrene	85-01-8	91.76	3.73	91.11	2.24	90.97	1.51	91.19	2.39
Pyrene	129-00-0	93.65	1.67	91.00	0.97	94.04	2.47	93.87	2.26
Pyrene-D10 (surr)	1718-52-1	96.28	3.53	94.75	1.54	95.11	1.70	95.35	2.80

Table 5. PCBs

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
2-Chlorobiphenyl	2051-60-7	90.04	2.77	90.94	2.61	89.65	1.73	89.73	2.41
2,3-Dichlorobiphenyl	16605-91-7	93.17	1.82	93.18	2.65	92.39	2.71	93.83	3.44
2,4,5-Trichorobiphenyl	15862-07-4	89.50	3.03	86.72	3.24	88.69	2.30	86.77	3.66
2,2,4,4-Tetrachlorobiphenyl	2437-79-8	93.04	2.99	89.83	2.81	91.64	2.10	88.11	3.27
2,2,3,4,6-Pentachlorobiphenyl	60233-25-2	85.24	2.61	82.48	3.00	85.62	1.94	80.50	3.23
2,2,4,4,5,6-Hexachlorobiphenyl	60145-22-4	85.15	2.50	83.70	3.61	85.95	2.10	81.30	3.12
2,2,3,3,4,4,6-Heptachlorobiphenyl	52663-71-5	85.84	2.69	86.77	2.92	87.09	2.48	86.10	2.37
2,2,3,3,4,5,6,6-Octachlorobiphenyl	40186-71-8	83.97	2.80	85.50	1.54	86.01	2.96	87.60	2.75
Decachlorobiphenyl	2051-24-3	81.96	2.55	87.74	2.14	83.50	3.56	90.15	1.82

Table 6. Other SVOCs

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
1,3 dimethyl-2-nitrobenzne (surr)	81-20-9	91.05	5.4	90.95	1.74	87.55	5.06	87.79	2.4
2,4-Dinitrotoluene	121-14-2	105.04	3.03	104.14	4.76	105.51	3.19	110.23	4.95
2,6-Dinitrotoluene	606-20-2	97.11	3.48	96.59	3.4	96.64	3.51	96.72	3.96
4,4-DDD	72-54-8	96.68	3.22	94.09	2.65	94.48	2.18	90.62	3.69
4,4-DDE	72-55-9	87.81	2.47	85.74	3.09	88.86	1.7	83.48	4.18
4,4-DDT	50-29-3	95.42	3.09	92.37	2.68	95.88	2.01	90.48	2.82
Ametryn	834-12-8	97.19	2.89	97.68	2.06	94.56	2.02	97.62	2.71
Atraton	1610-17-9	88.07	2.6	99.82	2.72	77.35	5.11	100.78	2.76

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Benzyl Butyl phthalate	85-68-7	124.79	2.9	122.76	3.29	118.41	2.65	119.6	3.78
Bromacil	314-40-9	112.05	2.81	111.06	2.56	108.31	2.18	108.47	1.81
Butylate	2008-41-5	93.9	2.65	94.25	2.17	92.46	1.87	92.5	2.59
Chlorobenzilate	510-15-6	107.17	3.4	107.08	2.33	106.44	1.67	108.39	2.92
Chloroneb	2675-77-6	92.62	5.67	92.88	5.16	94.54	2.42	93.71	2.82
Chlorothalonil	1897-45-6	98.3	2.5	96.39	2.57	97.49	1.48	97.18	2.77
Chlorpropham	101-21-3	106.16	1.5	105.64	3.28	103.89	1.87	106.13	2.58
Chlorpyrifos	2921-88-2	99.65	3.15	97.97	1.53	98.41	2.55	97.86	3.01
cis-Permethrin	61949-76-6	110.91	4.05	111.88	3.46	112.66	2.98	110.41	3.6
Cyanazine	21725-46-2	102.54	3.24	102.61	2.19	98.54	2	101.81	2.62
Cycloate	1134-23-2	96.12	2.39	96.2	2.34	95.12	1.77	94.79	2.35
Dacthal	1861-32-1	96.14	2.56	94.49	2.31	94.95	2.08	94.12	2.52
Dichlorvos	62-73-7	99.92	1.86	99.09	2.77	95.36	2.68	95.49	2.9
Diethylphthalate	84-66-2	100.82	2.45	100.51	3	98.96	2.59	98.68	3.06
Dimethylphthalte	131-11-3	98.85	1.98	97.3	2.97	96.34	2.33	96.31	2.96
Di-n-butylphthalate	84-74-2	120.72	5.23	120.65	3.63	115.92	5.08	116.83	5.07
Di-n-octyl phthalate	117-84-0	101.64	4.14	108.24	3.29	103.15	3.48	110.9	2.53
Diphenamid	957-51-7	100.18	2.84	98.32	2.25	98.19	1.81	97.89	2.63
Disulfoton Sulfone	2497-06-5	111.41	4.22	113.28	3.32	108.72	1.58	115	2.98
Endosulfan I	959-98-8	97.6	2.87	95.52	2.72	96.28	2.01	95.72	2.59
Endosulfan II	33213-65-9	98.95	2.65	97.94	1.78	98.11	1.53	98.06	2.51
Endosulfan Sulfate	1031-07-8	105.03	3.12	103.8	2.23	103.85	1.15	104.42	2.64
Endrin Aldehyde	7421-93-4	101.23	3.95	89.39	5.33	101.22	1.7	97.43	3.31
Endrin Ketone	53494-70-5	100.44	4.37	100.79	4.61	102.29	8.27	97.66	4.88
EPTC	759-94-4	94.21	2.39	94.76	2.49	92.96	1.9	92.3	2.6
Ethoprophos	13194-48-4	101.13	2.45	100.98	2.79	99.61	2.23	99.63	2.73
Etridiazole	2593-15-9	96.76	2.96	96.23	2.72	97.99	1.65	97.6	2.18
Fenarimol	60168-88-9	117.54	2.53	117.07	2.47	117.66	2.42	117.95	3.01
Hexazinone	51235-04-2	107.77	2.92	108.33	2.65	105.5	1.82	107.33	2.02
Isophorone	78-59-1	92.71	3.74	91.32	3.34	88.28	2.43	88.64	2.03
Methyl paraoxon	950-35-6	94.52	4.63	98.15	1.88	95.45	4.44	99.61	3.7
Metolachlor	51218-45-2	103.49	2.97	102.41	2.36	101.57	1.96	102.05	2.31
Mevinphos	7786-34-7	98.04	2.57	97.62	3.58	94.61	3.08	95.49	2.7
MGK-264 A	113-48-4	104.68	3.2	104.14	2.27	103.51	1.83	103.21	2.77
MGK-264 B	113-48-4	109.21	2.77	109.07	2.36	106.29	2.28	107.53	2.65
Molinate	2212-67-1	95.25	2.56	95.29	2.27	94.07	1.6	93.85	2.27
Naphthalene	91-20-3	95.31	3.49	93.59	2.78	93.54	1.78	91.02	2.54
Napropamide	15299-99-7	107.36	4.9	107.61	2.31	105.34	1.57	108.29	2.53

Analyte	CAS #	SPE-03				Presto			
		525.2		525.3		525.2		525.3	
		Average	RSD (%)	Average	RSD (%)	Average	RSD (%)	Average	RSD (%)
Norflurazon	27314-13-2	115.4	3.29	115.47	2.59	114.73	2.18	117.08	3.1
Pebulate	1114-71-2	90.5	1.35	91.9	1.29	93.66	2.63	94.75	2.58
Pentachlorophenol	87-86-5	93	3.36	94.64	1.99	91.76	2.05	95.3	2.45
Perylene-d12 (surr)	1520-96-3	93.16	4.03	92.54	2.24	93.24	1.71	91.17	3.21
Phenanthrene	85-01-8	91.76	3.73	91.11	2.24	90.97	1.51	91.19	2.39
Prometon	1610-18-0	95.39	3.61	97.64	2.28	90.39	2.4	97.31	2.54
Prometryn	7287-19-6	98.5	3.04	99.84	1.93	97.08	1.43	99.65	2.76
Pronamide	23950-58-5	100.45	3.38	99.81	1.66	98.47	1.86	99.37	2.43
Propazine	23950-58-5	97.25	2.17	96.55	2.22	96.99	1.66	97.25	2.36
Simetryn	1014-70-6	97.32	3.08	101.65	1.98	89.95	2.98	100.74	3.93
Tebuthiuron	34014-18-1	102.91	3.84	102.64	3.05	100.24	2.2	101.91	2.84
Terbacil	5902-51-2	102.71	3.23	101.98	3.04	98.92	1.62	100.27	2.55
Terbufos	13071-79-9	77.12	9.31	85.67	1.77	77.51	4.47	79.64	3.73
Terbutryn	886-50-0	100.53	3.39	101.15	2.1	99.15	1.3	101.14	2.99
Tetrachlorvinphos	22248-79-9	110.64	3.57	116.04	3.42	108.72	1.85	117.9	2.24
trans-Permethrin	61949-77-7	108.26	3.05	108.23	3.31	111.27	2.64	106.86	3.18
Triademefon	43121-43-3	99.84	2.77	98.47	1.9	98.48	1.82	98.16	2.6
Tricyclazole	41814-78-2	117.93	4.57	122.39	4.15	116.24	2.03	125.83	6.79
Trifluralin	1582-09-8	89.93	3.71	86.77	2.97	91.07	1.59	87.96	2.69
Triphenyl phosphate (surr)	115-86-6	106.15	3	105.09	2.5	104.41	1.44	104.77	2.72
Vernolate	1929-77-7	92.62	2.32	92.76	2.46	92.46	1.65	92.12	2.36

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