Environmental Applications note cat.# 59557

SPE Extraction for EPA Method 525.1

EPA Method 525.1 Overview

EPA Method 525.1 is used for the determination of organic compounds in drinking water by liquid-solid extraction and capillary column gas chromatograph/mass spectrometry. It is applicable to a wide range of organic compounds that are efficiently partitioned from the water sample onto a C18 organic phase chemically bonded to a solid silica matrix in a cartridge or disk.

SIMDisk[™]-GF extraction disks can be used in EPA Method 525.1

This procedure was followed to demonstrate method equivalency:

Sample Pretreatment:

Allow 1 liter of deionized water to equilibrate to room temperature in a narrow-mouth amber glass bottle. Adjust sample pH to less than 2 with 6M hydrochloric acid, being careful not to over acidify the sample. Addition of too much HC₁ can cause the formation of acidic extracts.

Apparatus Assembly:

Assemble the 47mm apparatus. Place the SIMDisk[™]-GF disk in the Diskcover[™]-47 filter support, wrinkled side up.

J Disk Precleaning:

Add 5ml of methylene chloride to the top surface of the disk and immediately draw through under vacuum at 15 in. Hg (50 kPa). Continue to draw vacuum at 15 in. Hg (50 kPa) for 5 minutes to remove all solvent.

4Disk Conditioning:

Add 5ml methanol to the top surface of the disk and immediately apply low vacuum (1- 2 in. Hg, 3-7 kPa). Draw through until the top surface of the methanol is just above the disk. Do not allow any air to pass through the disk or reach the top surface of the disk. Immediately add 5ml of deionized water to the disk and draw through at low vacuum until the water almost reaches the top surface of the disk. It is preferable to leave extra liquid above the disk rather than allow any air to contact the surface of the disk.

OSample Addition:

Add the sample onto the disk, directly to the film of water left from the conditioning step. Adjust the vacuum to 10 in. Hg (35 kPa) for a flow rate of approximately 100ml per minute until the entire sample has been passed through the disk.

Disk Drying:

After the sample has been processed, draw air through the disk under vacuum at approximately 15 in. Hg (50 kPa) for approximately 5 minutes.

Analyte Elution:

Release system vacuum. Insert the sample collection rack and collection vessels. Reassemble the apparatus. Add 5ml methylene chloride directly to the sample bottle and gently swirl to rinse all inner surfaces of the bottle. Allow the sample bottle to stand for 1 to 2 minutes and transfer the methylene chloride to the disk using a glass pipet. Rinse the reservoir sides in the process. Draw the solvent through the disk at 5 in. Hg (17 kPa). Repeat the bottle rinse and disk elution twice with fresh aliquots of methylene chloride, combining all eluates in the collection tube.

OFinal Analysis:

Remove water from sample eluate by passing it through approximately 3 grams of anhydrous sodium sulfate. Concentrate to 1ml and analyze 1µl by GC/MS.

> SIMDisk[™]-*GF*: cat.# 24004, 20-pack

EPA methods are available from the National Technical Information Service: 703-487-4650



Accuracy/Precision data from four determinations of Method 525.1 analytes at 2µg/L with Liquid-Solid SIMDisk[™]-GF 47mm extraction disk and the Finnigan MAT ITS40 Ion Trap MS

accmaphthalene-d10 5	compound	target conc. (µg/L)	mean (µg/L)	std. dev. (µg/L)	% RSD	accuracy (% of target)	% REC. in method
chrysene-dl25hexachlorocyclopentadiene21.60.302.18055anentyhtylene21.80.179.49095acenaphtylene22.00.603.1100952-chlorobiphenyl22.00.703.3105100flororene22.10.703.31051102,3-dichlorobiphenyl22.00.703.210085simazine21.90.1910.295110pentachlorophenol89.70.798.212197gamma-BHC22.10.401.2105110pentachlorophenol89.70.798.212197gamma-BHC22.20.401.9110120anthracene22.20.401.9110120anthracene22.10.401.7105heptachlor21.90.401.295151lein-burylphthalate22.50.249.5125110di-n-burylphthalate21.90.502.49595gamma-chlorodiphenyl21.90.502.49.5155gamma-chlorobiphenyl21.90.502.49595gamma-chlorobiphenyl21.70.502.89	acenaphthalene-d10	5					
hexachlorocyclopentadiene21.60.302.18055dimethylphthalate21.80.179490952-chlorobiphenyl22.00.603.1100952-chlorobiphenyl22.00.502.410095diethylphthalate22.10.703.31051102.3-dichlorobiphenyl22.00.703.21001153-dichlorobiphenyl22.00.602.810085simazine22.10.402.2105110petatachlorophenol89.70.798.212197gamma-BHC22.10.402.2105105phenathrene22.00.401.9110120anthracene22.00.401.9155853lachlor21.90.401.995853lachlor21.90.401.995110di-n-butylphthalate22.10.401.7105heptachlor exide (isomer B)21.60.201.29575aldrin21.60.201.295110di-n-butylphthalate22.10.502.49595gamma-chlorodiphenyl21.90.502.49595gamma-chlorodiphenyl21.90.502	henanthrene-d10	5					
dimethylphhalate 2 1.8 0.17 9.4 90 95 acenaphthylene 2 2.0 0.60 3.1 100 95 dicthylphthalate 2 2.0 0.50 2.4 100 95 dicthylphthalate 2 2.1 0.70 3.3 105 110 Provene 2 2.1 0.60 3.4 100 115 beachlorobenzene 2 2.0 0.60 2.8 100 85 simazine 2 1.9 0.19 10.2 95 105 atrazine 2 2.1 0.16 7.5 105 110 perman-BHC 2 2.1 0.40 1.9 110 120 antfracene 2 2.0 0.90 4.6 100 85 alachlor 2 1.9 0.40 1.9 95 152 1010 1.2 1.9 0.20 1.2 95	chrysene-d12	5					
accnaphilylene 2 2.0 0.60 3.1 100 95 2-chlorobiphenyl 2 2.0 0.50 2.4 100 95 dicthylphthalate 2 2.1 0.70 3.3 100 110 2.3-dichlorobiphenyl 2 2.0 0.70 3.2 100 115 hexachlorobenzene 2 2.0 0.60 2.8 100 85 simazine 2 1.9 0.19 10.2 95 105 attrazine 2 2.1 0.40 2.2 105 105 pentachlorophenol 8 9.7 0.79 8.2 121 97 gamma-BHC 2 2.2 0.40 1.9 100 120 anthracene 2 2.0 0.90 4.6 100 85 2.4,5-trichlorobiphenyl 2 1.9 0.40 1.7 105 aldrin 2 2.5 0.24 <t< td=""><td>hexachlorocyclopentadiene</td><td>2</td><td>1.6</td><td>0.30</td><td>2.1</td><td>80</td><td>55</td></t<>	hexachlorocyclopentadiene	2	1.6	0.30	2.1	80	55
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	dimethylphthalate	2	1.8	0.17	9.4	90	95
diethylphilatae22.10.703.3105100fluorene22.10.603.11051102.3-dichlorobiphenyl22.00.603.210085simazine21.90.1910.295105attrazine22.10.402.2105110pentachlorophenol89.70.798.212197gamma-BHC22.00.402.2105105phenanthrene22.00.904.6100852.4.5-trichlorobiphenyl21.90.401.99585alachlor21.90.401.99585alachlor21.90.402.295110di-n-butylphthalate22.50.249.51251102.2'.3'.4', etrachlorobiphenyl21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152.2'.3'.4', epentachlorobiphenyl21.90.502.4959595aldrin21.90.402.0100953152.2'.3'.4', epentachlorobiphenyl21.90.502.4951051152.2'.3'.4', epentachlorobiphenyl21.90.502.895100pyrne22.00.402.010095315 </td <td>acenaphthylene</td> <td>2</td> <td>2.0</td> <td>0.60</td> <td>3.1</td> <td>100</td> <td>95</td>	acenaphthylene	2	2.0	0.60	3.1	100	95
fluorene 2 2.1 0.60 3.1 105 110 2,3-dichlorobiphenyl 2 2.0 0.70 3.2 100 115 hexachlorobenzene 2 2.0 0.60 2.8 100 85 simazine 2 1.9 0.19 10.2 95 105 attrazine 2 2.1 0.16 7.5 105 110 pentachlorophenol 8 9.7 0.79 8.2 121 97 gamma-BHC 2 2.1 0.40 2.2 105 105 anthracene 2 2.0 0.90 4.6 100 85 2.4,5-trichlorobiphenyl 2 1.9 0.40 1.7 105 heptachlor 2 1.9 0.40 1.2 95 110 2.7,4,4-tetrachlorobiphenyl 2 1.6 0.20 1.2 95 115 2.7,2,4,4-tetrachlorobiphenyl 2 1.9 <td< td=""><td>2-chlorobiphenyl</td><td>2</td><td>2.0</td><td>0.50</td><td>2.4</td><td>100</td><td>95</td></td<>	2-chlorobiphenyl	2	2.0	0.50	2.4	100	95
2,3-dichlorobiphenyl22,00.703.2100115hexachlorobenzene22,00.602.810085simazine21,90,1910.295105attrazine22,10,167.5105110pentachlorophenol89,70.798.212197gamma-BHC22,20,401.9110120anthracene22,20,401.995852,4,5-trichlorobiphenyl21.90,401.99585alachlor22,10,401.7105heptachlor21.90,402.295110di-n-butylphthalate22.50,249.5125110 $2,2',4,4'$ -tetrachlorobiphenyl21.60.2012.78080heptachlor21.90,502.4959595gamma-chlorane21.90,502.495115 $2,2',3',4,6',6-hacklorobiphenyl21.70,14808580heptachlore21.90,502.495135gamma-chlorane21.90,502.895100pyrene20.60.402.010095gamma-chlorane21.90,502.8951352,2',3,3',4',5,6'-catchlorobiphenyl21.7$	diethylphthalate	2	2.1	0.70	3.3	105	100
hexachlorobenzne22.00.602.810085simazine21.90.1910.295105atrazine22.10.167.5105110pentachlorophenol89.70.798.212197gamma-BHC22.10.402.2105105phenanthrene22.20.401.9110120anthracene22.00.904.6100852,4,5-trichlorobiphenyl21.90.401.99585alachlor22.10.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.5125110 $2,2,4,4$ -tertachlorobiphenyl21.60.201.29575aldrin21.60.201.295115 $2,2,3,4,5$ -pentachlorobiphenyl21.90.502.49595gamma-chlor ance21.90.502.895110pyrene22.00.400.00095alpha-chlorobaphenyl21.70.148.085endrin22.20.502.895100trans-nonachlor21.90.703.795135 $2,2,4,4,5,6$ -hexachlorobiphenyl21.70.148.085	fluorene	2	2.1	0.60	3.1	105	110
simazine21.90.1910.295105attazine22.10.167.5105110pentachlorophenol89.70.798.212197gamma-BHC22.10.402.2105105phenanthrene22.20.401.9110120anthracene22.00.904.6100852.4,5-trichlorobiphenyl21.90.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.51251102.2,4,4-trachlorobiphenyl21.90.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152.2,3,4,4-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.502.895100pyrne22.00.402.010095alpha-chlordane21.90.502.895105jatharene22.20.502.211090bit(2-ettylhexylbathalate22.20.502.2110902.2,2,4,4',5,6'-hexachlorobiphenyl21.70.148.08580earma-klor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl	2,3-dichlorobiphenyl	2	2.0	0.70	3.2	100	115
atrazine 2 2.1 0.16 7.5 105 110 pentachlorophenol 8 9.7 0.79 8.2 121 97 gamma-BHC 2 2.1 0.40 2.2 105 105 phenanthrene 2 2.2 0.40 1.9 110 120 anthracene 2 2.1 0.40 1.9 95 85 alachlor 2 1.9 0.40 1.7 105 heptachlor 2 1.9 0.40 2.2 95 110 di-n-butylphthalate 2 2.5 0.24 9.5 125 110 2,2',4,4'-tetrachlorobiphenyl 2 1.6 0.20 12.7 80 80 heptachlor epoxide (isomer B) 2 2.1 0.50 2.5 105 115 gamma-Chordnane 2 1.9 0.80 4.1 95 135 2,2',4,5,6'-hexachlorobiphenyl 2 1.7	hexachlorobenzene	2	2.0	0.60	2.8	100	85
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	simazine	2	1.9	0.19	10.2	95	105
gamma-BHC22.10.402.2105phenanthrene22.20.401.9110120anthracene22.00.904.610085 $2,4,5$ -trichlorobiphenyl21.90.401.99585alachlor22.10.401.7105heptachlor21.90.402.295110 $di-n-butylphthalate22.50.249.51251102,2',4,4'-tetrachlorobiphenyl21.90.201.29575aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152,2',3',4.6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.502.895100pyrene22.00.402.010095alpha-chlordane21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.125.4110100bitg(2-ethylhexylphthalate22.20.125.4110100bitg(2-ethylhexylphthalate22.20.125.49090chroin22.20.125.4110100bitg(2-ethylhexylphthalate2<$	atrazine	2	2.1	0.16	7.5	105	110
ghenanthrene22.20.401.9110120anthracene22.00.904.6100852.4.5-trichlorobiphenyl21.90.401.7105heptachlor22.10.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.5125110 $2,2',4,4'$ -tetrachlorobiphenyl21.90.201.29575aldrin21.60.201.278080heptachlor epxide (isomer B)22.10.502.5105115 $2,2',3',4,6$ -pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.502.895100trans-nonachlor21.90.703.795135 $2,2',3',4,6'$ -betachlorobiphenyl21.70.148.08580endrin22.20.502.21109090butylbenzylphthalate22.10.502.510590 $2,2',3,3',4,4',6'-heptachlorobiphenyl21.70.201.28590butylbenzylphthalate22.20.125.4110100bis(2-ethylhexylphthalate22.10.502.5105902,2',3,3',4,4',6,6'-octachlorobiphenyl21.70.20$	pentachlorophenol	8	9.7	0.79	8.2	121	97
anthracene22.00.904.6100852.4,5-trichlorobiphenyl21.90.401.99585alachlor22.10.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.51251102.2,2,4,4'-tetrachlorobiphenyl21.90.201.29575aldrin21.60.201.29595gamma-chlorobiphenyl21.90.502.49595gamma-chlordane21.90.502.49595gamma-chlordane21.90.703.7951352.2', 4, 4, 5, 6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.21109090bis(2-ethylhexylphthalate22.20.502.2110902.2', 3, 3, 4, 4'-6-heptachlorobiphenyl21.80.401.99070methoxychlor21.90.200.995110bis(2-ethylhexylphthalate22.20.502.5105902.2', 3, 3, 4, 4'-6-heptachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.0	gamma-BHC	2	2.1	0.40	2.2	105	105
2.4,5-trichlorobiphenyl21.90.401.99585alachlor22.10.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.5125110 $2.2,4,4'$ -tetrachlorobiphenyl21.90.201.29575aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.49595gamma-chlorane21.90.804.195110pyrene22.00.402.010095alpha-chlorane21.90.502.895100trans-nonachlor21.90.703.795135 $2.2,4,4',5,6'$ -hexachlorobiphenyl21.70.148.08580endrin22.20.502.21109090butylbenzylphthalate22.20.502.510590 $2,2',3,3',4,4',6-hetxachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,4',6-hetxachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,4',6-hetxachlorobiphenyl21.70.201.285$	phenanthrene	2	2.2	0.40	1.9	110	120
alachlor22.10.401.7105heptachlor21.90.402.295110di-n-butylphthalate22.50.249.51251102,2',4,4'-tetrachlorobiphenyl21.90.201.29575aldrin21.60.201.28080heptachlor epoxide (isomer B)22.10.502.51051152,2',3',4,6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyladipate21.80.401.99070methoxychlor22.10.502.510590c,13,3,4,4',6-heptachlorobiphenyl21.70.200.28590benzo(a)anthracene21.90.200.99590c,hrysne21.90.200.99590benzo(b)fluoranthene22.00.904.2100benzo(b)fluorant	anthracene	2	2.0	0.90	4.6	100	85
heptachlor21.90.402.295110di-n-butylphthalate22.50.249.51251102,2',4,4'-tetrachlorobiphenyl21.90.201.29575aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152,2',3',4,6-pentachlorobiphenyl21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995902,2',3,3',4,5',6,6'-octachlorobiphenyl21.90.200.99590chrosene <t< td=""><td>2,4,5-trichlorobiphenyl</td><td>2</td><td>1.9</td><td>0.40</td><td>1.9</td><td>95</td><td>85</td></t<>	2,4,5-trichlorobiphenyl	2	1.9	0.40	1.9	95	85
di-n-butylphthalate22.50.249.51251102,2',4,4'-tetrachlorobiphenyl21.90.201.29575aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152,2',3',4,6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.99590chrysene21.90.200.99590chrysene22.00.904.2100benzo(b)fluoranthene22.00.904.2100benzo(b)fluoranthene22.00.804.2100benzo(b)fluoranthene22.00.909590110	alachlor	2	2.1	0.40	1.7	105	
2.2;4,4'-tetrachlorobiphenyl 2 1.9 0.20 1.2 95 75 aldrin 2 1.6 0.20 12.7 80 80 heptachlor epoxide (isomer B) 2 2.1 0.50 2.5 105 115 2,2',3',4,6-pentachlorobiphenyl 2 1.9 0.50 2.4 95 95 gamma-chlordane 2 1.9 0.80 4.1 95 110 pyrene 2 2.0 0.40 2.0 100 95 alpha-chlordane 2 1.9 0.70 3.7 95 135 2,2',4,4',5,6'-hexachlorobiphenyl 2 1.7 0.14 8.0 85 80 endrin 2 2.2 0.50 2.2 110 90 butylbenzylphthalate 2 2.2 0.50 2.2 110 90 butylbenzylphthalate 2 1.8 0.21 11.9 90 80 2,2',3,3',4,4',6-heptachlorobiphenyl 2 1.7 0.20 0.9 95 90 chrysene<	heptachlor	2	1.9	0.40	2.2	95	110
aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152.2',3',4,6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352.2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate21.80.2111.990802.2',3,3',4,4',6-heptachlorobiphenyl21.70.201.28590 $2,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.285902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995110benzo(a)anthracene21.90.200.995110bis(2-ethylhexylphthalate22.20.402.011095benzo(k)fluoranthene22.00.804.2100benzo(k)fluoranthene22.00.105.110040perylene-d1254.7$	di-n-butylphthalate	2	2.5	0.24	9.5	125	110
aldrin21.60.2012.78080heptachlor epoxide (isomer B)22.10.502.51051152.2',3',4,6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352.2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate21.80.2111.990802.2',3,3',4,4',6-heptachlorobiphenyl21.70.201.28590 $2,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.285902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.200.995110benzo(a)anthracene21.90.200.995110bis(2-ethylhexylphthalate22.20.402.011095benzo(k)fluoranthene22.00.804.2100benzo(k)fluoranthene22.00.105.110040perylene-d1254.7$	2,2',4,4'-tetrachlorobiphenyl	2	1.9	0.20	1.2	95	75
2,2',3',4,6-pentachlorobiphenyl21.90.502.49595gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(k)fluoranthene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.6	aldrin	2	1.6	0.20	12.7	80	80
gamma-chlordane21.90.804.195110pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.401.990802,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.202.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(k)fluoranthene22.00.804.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)prene22.00.804.210040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	heptachlor epoxide (isomer B)	2	2.1	0.50	2.5	105	115
pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.401.990802,2',3,3',4,4',6-heptachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(k)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	2,2',3',4,6-pentachlorobiphenyl	2	1.9	0.50	2.4	95	95
pyrene22.00.402.010095alpha-chlordane21.90.502.895100trans-nonachlor21.90.703.7951352,2',4,4',5,6'-hexachlorobiphenyl21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.401.990802,2',3,3',4,4',6-heptachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(k)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	gamma-chlordane	2	1.9	0.80	4.1	95	110
trans-nonachlor21.90.703.795135trans-nonachlor21.70.148.08580endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,4',6-heptachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.285902,2',3,3',4,5',6,6'-octachlorobiphenyl21.90.200.995110benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.00.402.011095benzo(a)anthracene21.90.200.995110bis(2-ethylhexyl)phthalate22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(k)fluoranthene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	2.0	0.40	2.0	100	95
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	alpha-chlordane	2	1.9	0.50	2.8	95	100
endrin22.20.502.211090butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,4',6-heptachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.285902,2',3,3',4,5',6,6'-octachlorobiphenyl21.90.200.99590chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(k)fluoranthene22.00.804.2100benzo(k)fluoranthene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	trans-nonachlor	2	1.9	0.70	3.7	95	135
butylbenzylphthalate22.20.125.4110100bis(2-ethylhexyl)adipate21.80.2111.990802,2',3,3',4,4',6-heptachlorobiphenyl21.80.401.99070methoxychlor22.10.502.5105902,2',3,3',4,5',6,6'-octachlorobiphenyl21.70.201.28590 $2,2',3,3',4,5',6,6'-octachlorobiphenyl21.90.200.99590chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520$	2,2',4,4',5,6'-hexachlorobiphenyl	2	1.7	0.14	8.0	85	80
bis(2-ethylhexyl)adipate 2 1.8 0.11 1.19 90 80 2,2',3,3',4,4',6-heptachlorobiphenyl 2 1.8 0.40 1.9 90 70 methoxychlor 2 2.1 0.50 2.5 105 90 2,2',3,3',4,5',6,6'-octachlorobiphenyl 2 1.7 0.20 1.2 85 90 2,2',3,3',4,5',6,6'-octachlorobiphenyl 2 1.7 0.20 0.9 95 90 chrysene 2 1.9 0.20 0.9 95 110 bis(2-ethylhexyl)phthalate 2 2.2 0.40 2.0 110 95 benzo(b)fluoranthene 2 2.0 0.90 4.2 100 benzo(k)fluoranthene 2 2.0 0.80 4.2 100 105 benzo(a)pyrene 2 2.0 0.10 5.1 100 40 perylene-d12 5 4.7 0.34 7.3 94 100 indeno(1,2,3-cd)pyrene 2 1.9 0.22 11.6 95 20	endrin	2	2.2	0.50	2.2	110	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	butylbenzylphthalate	2	2.2	0.12	5.4	110	100
methoxychlor 2 2.1 0.50 2.5 105 90 2,2',3,3',4,5',6,6'-octachlorobiphenyl 2 1.7 0.20 1.2 85 90 benzo(a)anthracene 2 1.9 0.20 0.9 95 90 chrysene 2 1.9 0.20 0.9 95 110 bis(2-ethylhexyl)phthalate 2 2.2 0.40 2.0 110 95 benzo(k)fluoranthene 2 2.0 0.90 4.2 100 benzo(k)fluoranthene 2 2.0 0.80 4.2 100 105 benzo(k)fluoranthene 2 2.0 0.10 5.1 100 40 perylene-d12 5 4.7 0.34 7.3 94 100 indeno(1,2,3-cd)pyrene 2 1.9 0.22 11.6 95 20	bis(2-ethylhexyl)adipate	2	1.8	0.21	11.9	90	80
Initial constraintImage: constraint constraintImage: constraint constraintImage: constraint constraintImage: constraint constraint $2,2',3,3',4,5',6,6'$ -octachlorobiphenyl21.70.201.28590benzo(a)anthracene21.90.200.99590chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	2,2',3,3',4,4',6-heptachlorobiphenyl	2	1.8	0.40	1.9	90	70
benzo(a)anthracene21.90.200.99590chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	methoxychlor	2	2.1	0.50	2.5	105	90
chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	2,2',3,3',4,5',6,6'-octachlorobiphenyl	2	1.7	0.20	1.2	85	90
chrysene21.90.200.995110bis(2-ethylhexyl)phthalate22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	1.9	0.20	0.9	95	90
bis22.20.402.011095benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	1.9	0.20	0.9	95	110
benzo(b)fluoranthene22.00.904.2100benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	2.2	0.40	2.0	110	95
benzo(k)fluoranthene22.00.804.2100105benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	2.0	0.90	4.2	100	
benzo(a)pyrene22.00.105.110040perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520	· · ·	2			4.2		105
perylene-d1254.70.347.394100indeno(1,2,3-cd)pyrene21.90.2211.69520		2	2.0		5.1	100	
indeno(1,2,3-cd)pyrene 2 1.9 0.22 11.6 95 20	· · · · · ·						
benzo(g,h,i)perylene 2 1.8 0.18 9.9 90 35							

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