

WELLINGTON LABORATORIES

Reference and Handling Guide

GC/MS CHARACTERIZATION AND ANALYSIS OF
SELECTED HALOGENATED AROMATIC COMPOUNDS



A
USEFUL
GUIDE
ON
THE
ROAD
TO
SUCCESS

GUIDELINES FOR THE USE AND HANDLING OF WELLINGTON PRODUCTS

HAZARDS

The majority of our products are solutions of halogenated aromatic hydrocarbons in organic solvents such as nonane, toluene and isoctane. Although the maximum concentration is 100 µg/mL, that is 0.01% (w/v), these compounds must be considered toxic and potentially carcinogenic and should be handled accordingly.

As with all of our products, due care should be exercised to prevent human contact and ingestion. The absence of a toxicity warning for any of our products must not be interpreted as an indication that there is no possible health hazard.



NOTE:

**THESE MATERIALS SHOULD ONLY BE USED
BY PERSONNEL TRAINED IN THE HANDLING
OF HAZARDOUS CHEMICALS.
ALL PROCEDURES SHOULD BE PERFORMED
IN A FUME HOOD AND SUITABLE GLOVES,
EYE PROTECTION AND CLOTHING SHOULD
BE WORN AT ALL TIMES.**

RECEIPT, INSPECTION, HANDLING AND STORAGE

Unless crystalline material is provided, all of our reference standard solutions are shipped in flame-sealed, pre-scored amber glass ampoules. Upon receipt, inspect the ampoules for breakage and leakage and then store them upright until needed. The ampoules can be stored at ambient temperature until opened.

Prior to opening, allow the solution to drain into the bottom of the ampoule, lightly tapping the ampoule if necessary. Using the plastic ampoule collar provided, hold the ampoule upright and snap the top off, breaking away from the body.

Transfer the solution to an amber glass container that can be tightly sealed for storage. To prevent evaporation of the solvent, it is suggested that this solution, and subsequent mixtures and/or dilutions, be stored at refrigerator temperatures.

DISPOSAL

All waste materials generated during the use of these solutions should be treated as hazardous in accordance with national and regional regulations. A licensed disposal company should be employed. Some options for the destruction of these materials include high temperature incineration, photolysis or chemical treatment using reagents such as sodium naphthalene or KPEG reagent. Literature references for some of these methods can be provided upon request.

ACCURACY

Each of our stock solutions is prepared from crystalline material that has been well characterized as to its structure and purity.

The crystalline material is weighed using microbalances that are externally calibrated and traceable to an ISO/IEC 17025 accredited laboratory. Solutions are prepared by completely dissolving the crystalline material in ultrapure, distilled-in-glass solvents. The volumetric flasks used for this purpose, and the pipets used for subsequent preparation of dilutions and mixtures, are all of class A tolerance and traceable to an ISO/IEC 17025 accredited laboratory.

The maximum percent relative combined uncertainty for solution preparation is calculated to be $\pm 5\%$.

INTERLABORATORY CERTIFICATION

Wellington continues to submit its standards for independent interlaboratory testing and certification. Since 1991, our standards have been tested in over 20 international round-robbins.

To date, solutions of the compounds listed below have been repeatedly tested and the approximate total number of analyses are given.

- 2,3,7,8-substituted PCDDs and PCDFs.....1700 HRMS analyses
- Dioxin-like (WHO) PCB congeners.....1200 HRMS analyses
- PBDEs350 HRMS analyses

The overall averages of the data received for all of the compounds were found to be well within $\pm 10\%$ of the design values.

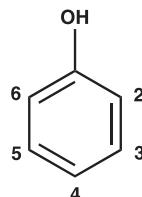
EXPIRY DATE/SHELF LIFE

In order to accurately determine the shelf life of our products, testing must reveal significant degradation or loss in concentration of the particular analyte. In comparing freshly prepared solutions to older solutions by GC/MS, we have not detected any significant changes. Many of these older solutions were prepared and ampouled more than 15 years ago. Thus our stability studies, as they should, remain ongoing.

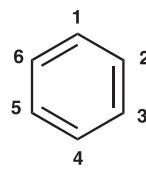
For our products where the expiry date on the certificate of analysis (CoA) states, "stability studies ongoing", we consider that our reference standard solutions retain their accuracy for a period of 5 years from delivery in the unopened ampoule.

NOTE: The predominant degradation pathway for our compounds is likely photolysis and thus protection from light is critical.

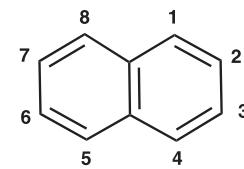
General Structure and Numbering System of Selected Aromatic Hydrocarbons



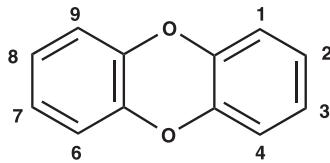
phenol



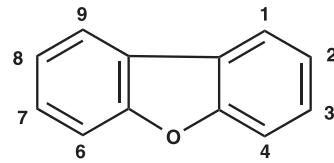
benzene



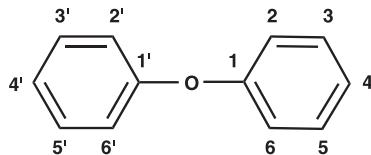
naphthalene



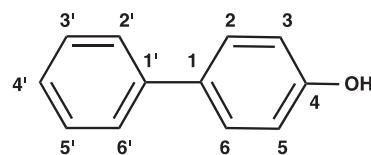
dibenzo-*p*-dioxin



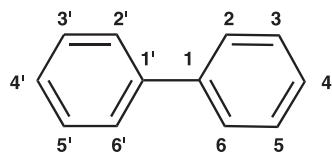
dibenzofuran



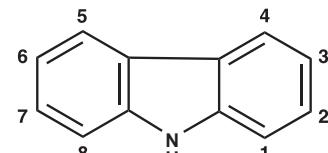
diphenyl ether



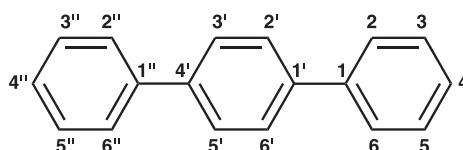
4-hydroxybiphenyl



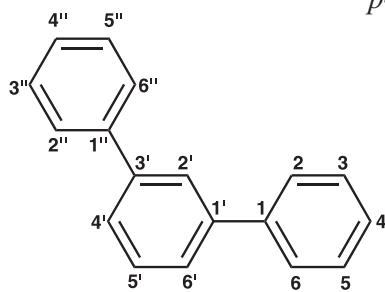
biphenyl



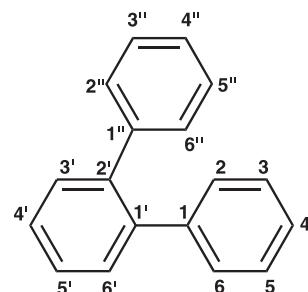
carbazole



p-terphenyl



m-terphenyl



o-terphenyl

Number of Possible Isomers for Selected Halogenated Aromatic Compounds

# of X	Terphenyl			Biphenyl	Biphenylol	Dibenz-p-dioxin	Dibenzofuran	Naphthalene	Benzene	Phenol
	ortho	meta	para							
1	5	6	4	3	19	2	4	2	1	3
2	28	28	21	12	64	10	16	10	3	6
3	80	87	55	24	136	14	28	14	3	6
4	211	211	139	42	198	22	38	22	3	3
5	355	382	226	46	198	14	28	14	1	1
6	544	544	351	42	136	10	16	10	1	
7	596	638	358	24	64	2	4	2		
8	544	544	351	12	19	1	1	1		
9	355	382	226	3	3					
10	211	211	139	1						
11	80	87	55							
12	28	28	21							
13	5	6	4							
14	1	1	1							

X = Halogen (does not apply to mixed halogenated compounds)

For diphenyl ethers use the biphenyl values

Molecular Weights for Selected Chlorinated and Brominated Aromatic Hydrocarbons

# of Cl/Br	PCTs	PCBs	PCDEs	PCDDs	PCDFs	PCNs	CBs	CPs	PBBS	PBDEs	PBDDs	PBDFs
0	230.31	154.21	170.21	184.19	168.19	128.17	78.11	94.11	154.21	170.21	184.19	168.19
1	264.75	188.66	204.66	218.64	202.64	162.62	112.56	128.56	233.11	249.11	263.09	247.09
2	299.20	223.10	239.10	253.08	237.09	197.06	147.00	163.00	312.00	328.00	341.99	325.99
3	333.64	257.55	273.55	287.53	271.53	231.51	181.45	197.45	390.90	406.90	420.88	404.88
4	368.09	291.99	307.99	321.97	305.98	265.95	215.89	231.89	469.80	485.80	499.78	483.78
5	402.53	326.44	342.44	356.42	340.42	300.40	250.34	266.34	548.69	564.69	578.67	562.68
6	436.98	360.88	376.88	390.86	374.87	334.84	284.78		627.59	643.59	657.57	641.57
7	471.42	395.33	411.33	425.31	409.31	369.29			706.48	722.48	736.47	720.47
8	505.87	429.77	445.77	459.75	443.76	403.73			785.38	801.38	815.36	799.36
9	540.31	464.22	480.22						864.28	880.28		
10	574.76	498.66	514.66						943.17	959.17		
11	609.20											
12	643.65											
13	678.09											
14	712.54											

Note: The molecular weight for PCHBs ($C_{12}H_{9-n}Cl_nOH$) is the same as the PCDEs ($C_{12}H_{10-n}Cl_nO$), but the maximum # of chlorines is one less for the PCHBs.

PCTs = polychlorinated terphenyls, PCBs = polychlorinated biphenyls, PCDEs = polychlorinated diphenyl ethers
PCHBs = polychlorinated hydroxybiphenyls (biphenylols), PCDDs = polychlorinated dibenz-p-dioxins,
PCDFs = polychlorinated dibenzofurans, PCNs = polychlorinated naphthalenes, CBs = chlorobenzenes, CPs = chlorophenols,
PBBS = polybrominated biphenyls, PBDEs = polybrominated diphenyl ethers,
PBDDs = polybrominated dibenz-p-dioxins, PBDFs = polybrominated dibenzofurans

Exact Mass & Relative Ion Abundances of Selected Chlorinated Aromatic Hydrocarbons

# of Cl	PCDFs				PCNs			CBs			CPs		
	$^{12}\text{C}_{12}$	$\text{C}_{12}\text{H}_{8-n}\text{Cl}_n\text{O}$	$^{13}\text{C}_{12}$	$^{12}\text{C}_{10}$	$\text{C}_{10}\text{H}_{8-n}\text{Cl}_n$	$^{13}\text{C}_{10}$	$^{12}\text{C}_6$	$\text{C}_6\text{H}_{6-n}\text{Cl}_n$	$^{13}\text{C}_6$	$^{12}\text{C}_6$	$\text{C}_6\text{H}_{5-n}\text{Cl}_n\text{OH}$	$^{13}\text{C}_6$	
0	168.0575	100	180.0978	128.0626	100	138.0962	78.0470	100	84.0671	94.0419	100	100.0620	
1	202.0185	100	214.0588	162.0236	100	172.0572	112.0080	100	118.0281	128.0029	100	134.0230	
	204.0156	33.5	216.0559	164.0207	33.0	174.0542	114.0050	32.6	120.0252	129.9999	32.8	136.0201	
2	235.9796	100	248.0198	195.9847	100	206.0182	145.9690	100	151.9891	161.9639	100	167.9841	
	237.9766	65.8	250.0169	197.9817	65.4	208.0153	147.9661	65.0	153.9862	163.9610	65.2	169.9811	
	239.9737	11.2	252.0139	199.9788	10.9	210.0123	149.9631	10.6	155.9832	165.9580	10.8	171.9782	
3	269.9406	100	281.9809	229.9457	100	239.9792	179.9300	100	185.9502	195.9249	100	201.9451	
	271.9376	98.2	283.9779	231.9427	97.8	241.9763	181.9271	97.4	187.9472	197.9220	97.6	203.9421	
	273.9347	32.5	285.9750	233.9398	32.0	243.9733	183.9241	31.7	189.9443	199.9190	31.9	205.9392	
	275.9317	3.7	287.9720	235.9368	3.6	245.9704	185.9212	3.5	191.9413	201.9161	3.5	207.9362	
4	303.9016	76.5	315.9419	263.9067	76.8	273.9403	213.8911	77.1	219.9112	229.8860	76.9	235.9061	
	305.8987	100	317.9389	265.9038	100	275.9373	215.8881	100	221.9082	231.8830	100	237.9032	
	307.8957	49.2	319.9360	267.9008	49.0	277.9344	217.8852	48.7	223.9053	233.8801	48.8	239.9002	
	309.8928	10.9	321.9330	269.8979	10.7	279.9314	219.8822	10.6	225.9023	235.8771	10.7	241.8973	
5	337.8627	61.3	349.9029	297.8677	61.5	307.9013	247.8521	61.7	253.8722	263.8470	61.6	269.8671	
	339.8597	100	351.9000	299.8648	100	309.8983	249.8491	100	255.8693	265.8441	100	271.8642	
	341.8568	65.4	353.8970	301.8618	65.1	311.8954	251.8462	64.9	257.8663	267.8411	65.0	273.8612	
	343.8538	21.5	355.8941	303.8589	21.3	313.8924	253.8432	21.1	259.8634	269.8382	21.2	275.8583	
6	371.8237	51.2	383.8639	331.8288	51.3	341.8623	281.8131	51.4	287.8332				
	373.8207	100	385.8610	333.8258	100	343.8594	283.8102	100	289.8303				
	375.8178	81.6	387.8580	335.8229	81.3	345.8564	285.8072	81.1	291.8273				
	377.8148	35.6	389.8551	337.8199	35.3	347.8535	287.8043	35.1	293.8244				
7	405.7847	43.9	417.8250	365.7898	44.0	375.8233							
	407.7818	100	419.8220	367.7868	100	377.8204							
	409.7788	97.8	421.8191	369.7839	97.5	379.8174							
	411.7759	53.3	423.8161	371.7809	52.9	381.8145							
	413.7729	17.5	425.8132	373.7780	17.3	383.8115							
8	439.7457	33.7	451.7860	399.7508	33.9	409.7844							
	441.7428	87.7	453.7830	401.7479	87.9	411.7814							
	443.7398	100	455.7801	403.7449	100	413.7785							
	445.7369	65.2	457.7771	405.7420	65.0	415.7755							
	447.7339	26.7	459.7742	407.7390	26.5	417.7726							

PCTs = polychlorinated terphenyls

PCBs = polychlorinated biphenyls

PCHBs = polychlorinated hydroxybiphenyls

PCDDs = polychlorinated dibenz-p-dioxins

PCDFs = polychlorinated dibenzofurans

PCNs = polychlorinated naphthalenes

CBs = chlorobenzenes

CPs = chlorophenols

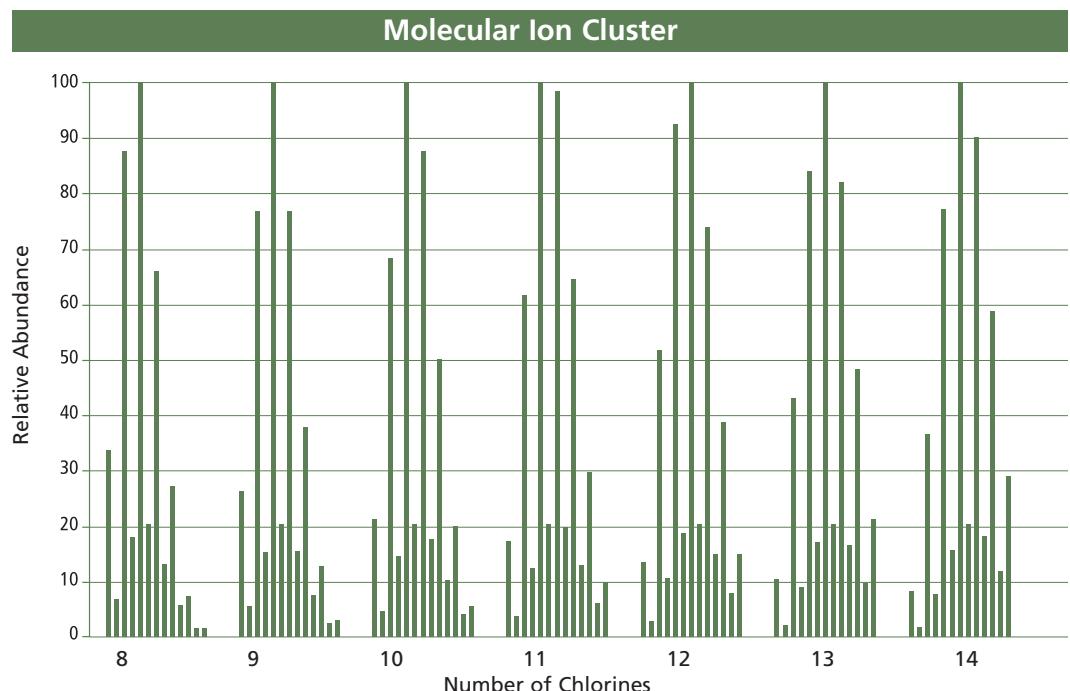
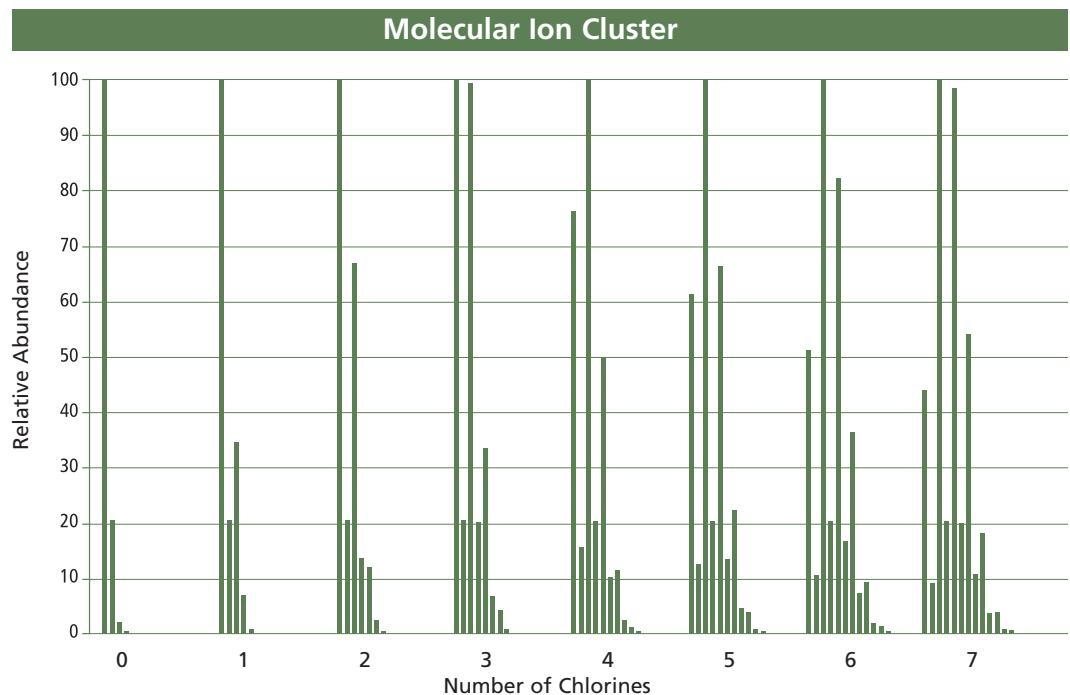
Accurate masses: $^{12}\text{C}=12.000000$, $^{13}\text{C}=13.003355$, $^1\text{H}=1.007825$, $^{35}\text{Cl}=34.968853$, $^{37}\text{Cl}=36.965903$, $^{16}\text{O}=15.994915$

Relative abundances of isotopes were determined using the method described in: Pretsch,Clerc,Seibl,Simon, Tables of Spectral Data for Structure Determination of Organic Compounds, Springer-Verlag, 1983.

The following natural isotopic abundances were used in all calculations: $^{12}\text{C}=98.89\%$, $^{13}\text{C}=1.11\%$, $^1\text{H}=99.985\%$, $^2\text{H}=0.015\%$, $^{35}\text{Cl}=75.53\%$, $^{37}\text{Cl}=24.47\%$, $^{16}\text{O}=99.759\%$, $^{17}\text{O}=0.037\%$, $^{18}\text{O}=0.204\%$.

Cl_n

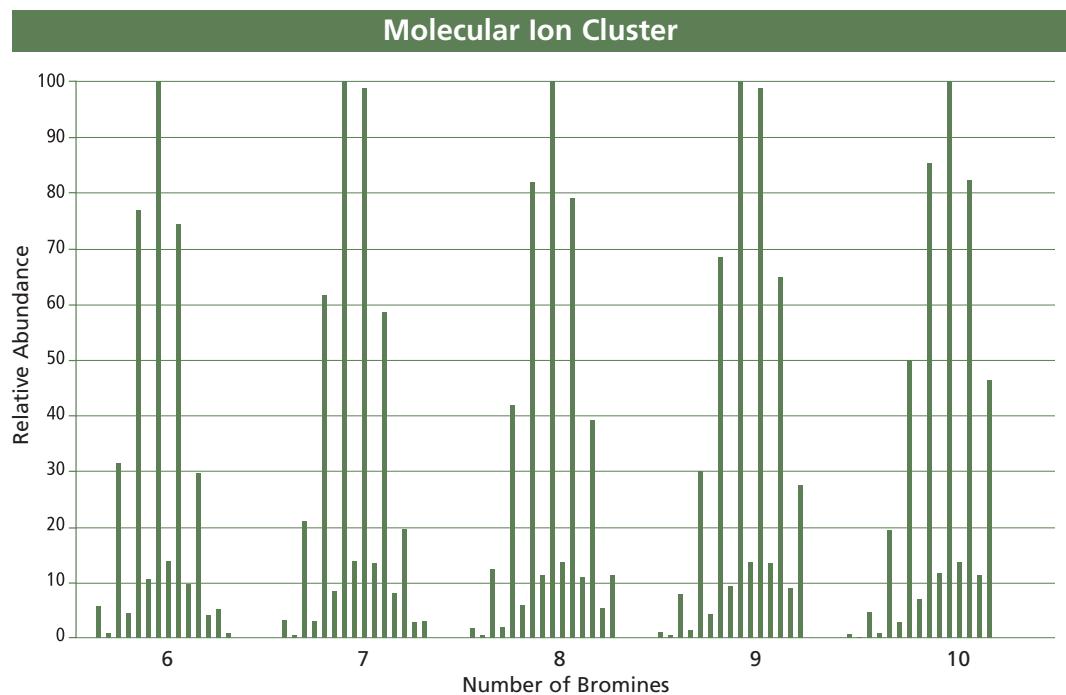
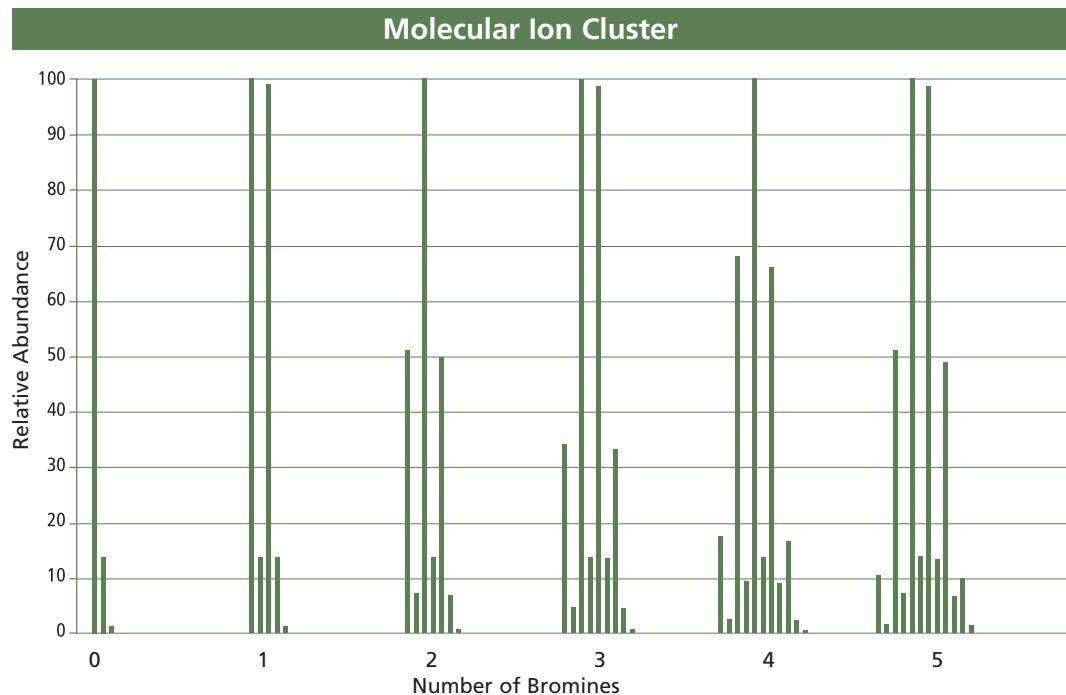
MOLECULAR ION CLUSTERS FOR CHLORINATED AROMATIC COMPOUNDS



Ions shown are M, M+1, M+2, M+3, M+4, M+5, M+6, M+7, M+8, M+9, M+10, M+11, M+12, and are representative of chlorinated terphenyls ($\text{C}_{18}\text{H}_{14-n}\text{Cl}_n$)

MOLECULAR ION CLUSTERS FOR BROMINATED AROMATIC COMPOUNDS

Br_n



Ions shown are M, M+1, M+2, M+3, M+4, M+5, M+6, M+7, M+8, M+9, M+10, M+11, M+12, M+13, M+14 and are representative of brominated diphenyl ethers ($\text{C}_{12}\text{H}_{10-n}\text{Br}_n\text{O}$)

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Standards for Environmental Testing and Research

Conversion Factors and Units of Measure

Prefix	Symbol	Factor	Fraction	
centi	c	10^{-2}	= 1/100	part per hundred
milli	m	10^{-3}	= 1/1,000	part per thousand
micro	μ	10^{-6}	= 1/1,000,000	part per million (ppm)
nano	n	10^{-9}	= 1/1,000,000,000	part per billion (ppb)
pico	p	10^{-12}	= 1/1,000,000,000,000	part per trillion (ppt)
femto	f	10^{-15}	= 1/1,000,000,000,000,000	part per quadrillion (ppq)
atto	a	10^{-18}	= 1/1,000,000,000,000,000,000	part per quintillion
zepto	z	10^{-21}	= 1/1,000,000,000,000,000,000,000	part per sextillion
yocto	y	10^{-24}	= 1/1,000,000,000,000,000,000,000,000	part per septillion

Commonly Used Units of Measure

wt/wt basis				wt/vol basis			
ppm	mg/kg	μ g/g	ng/mg	ppm	mg/L	μ g/mL	ng/ μ L
ppb	μ g/kg	ng/g	pg/mg	ppb	μ g/L	ng/mL	pg/ μ L
ppt	ng/kg	pg/g	fg/mg	ppt	ng/L	pg/mL	fg/ μ L
ppq	pg/kg	fg/g	ag/mg	ppq	pg/L	fg/mL	ag/ μ L





Standards for Environmental Testing and Research

Although a few items have been updated, this is essentially the fifth printing of our reference guide. As always, we continue to expand our inventory of compounds of potential environmental and/or toxicological concern. Rather than trying to include these emerging contaminants in this guide, we will prepare and post separate reference guides, specific to these new standards, on our website.

As before, if you have any comments or suggestions for future reference guides or if you would like to receive additional copies of this guide, please contact us at:

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