

The Standard

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INSIDE THIS ISSUE:

- CALL FOR USER-AUTHORED APPLICATION NOTES
PAGE 2
- NEW PRODUCTS
PAGE 3-4
- PAH UPDATE
PAGE 4
- NEW ¹³C PCBs
PAGE 5
- DIOXINS AND FURANS IN POLAR SOLVENTS
PAGE 5
- NITROSAMINES
PAGE 6
- LAKE APOPKA
PAGE 6
- PESTICIDE METABOLITE INITIATIVE
PAGE 6

Quality is
Always
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Solution

POLYBROMINATED Diphenyl Ethers - Environmental Contaminants of Concern

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Background

Brominated flame retardants (BFRs) include a large number of different types of brominated substances used extensively in polymers and textiles to prevent ignition and to slow down the initial phase of a developing fire. One class of BFRs is polybrominated diphenyl ethers (PBDEs), which are frequently used as additives in plastic materials for electronic and electrical goods and in textiles. The annual global consumption in 1992 of PBDEs was estimated to be 40,000 tons. PBDEs are commercially produced in mixtures with different degrees of bromination, with penta, octa and decaBDE corresponding to 10, 15 and 75 %, respectively, of the total PBDE consumption.

PBDEs were reported as environmental pollutants in pike from the Swedish river Viskan in 1981. Since then, PBDEs have been reported as pollutants in fish, birds, and mammals, as well as in sediments. The concentrations of BDE-47 have been reported to be approximately 2 ng/g (l.w.) both in human blood and in mothers' milk. It is alarming that the PBDE levels are increasing over time as have been shown in mothers' milk.

In biota, among all PBDE congeners, BDE-47 seems to be present at the highest concentrations. Other PBDE congeners found in the environment are 2,2',4,4',5-pentaBDE (BDE-99), 2,2',4,4',6-pentaBDE (BDE-100), 2,2',4,4',5,5'-hexaBDE (BDE-153), and 2,2',4,4',5,6'-hexaBDE (BDE-154). In addition, a heptaBDE has been identified in trout from Lake Ontario, USA. Typical levels in a few selected materials are summarized in Table 1.

Table 1. Concentrations (ng/g lipid weight (l.w.) of PBDEs in humans and wildlife.

Species	Locality	Tissue	PBDE concentration (ng/g l.w.)		
			BDE-47	BDE-99	BDE-100
Human	Sweden	Plasma	1.6	n.a.	n.a.
Human	Sweden	Milk	2.2	0.4	0.5
Salmon	Baltic Sea	Muscle	200	54	47
Herring	Bothnian Sea	Muscle	82	14	27
Grey seal	Baltic Sea	Blubber	650	38	40

continued on page 2

PBDE standards

PBDEs are commercially produced by direct bromination of diphenyl ether in the presence of a catalyst. Methods that are much more specific are in general necessary for the synthesis of pure individual PBDE standards. The standards listed in Table 2 are available from Cambridge Isotope Laboratories, Inc.

Table 2. PBDE congeners that have been synthesized. Compounds present in the commercial pentaBDE product, Bromkal 70-5DE, are given in bold italics.

BDE No.	No. of Br	Structure	BDE No.	No. of Br	Structure
1	1	2	47	4	2,2',4,4'
2	1	3	51	4	2,2',4,6'
3	1	4	66	4	2,3',4,4'
7	2	2,4	71	4	2,3',4',6
8	2	2,4'	75	4	2,4,4',6
10	2	2,6	77	4	3,3',4,4'
11	2	3,3'	85	5	2,2',3,4,4'
12	2	3,4	99	5	2,2',4,4',5
13	2	3,4'	100	5	2,2',4,4',6
15	2	4,4'	116	5	2,3,4,5,6
17	3	2,2',4	119	5	2,3',4,4',6
25	3	2,3',4	138	6	2,2',3,4,4',5'
28	3	2,4,4'	140	6	2,2',3,4,4',6'
30	3	2,4,6	153	6	2,2',4,4',5,5'
2	3	2,4',6	154	6	2,2',4,4',5,6'
33	3	2',3,4	155	6	2,2',4,4',6,6'
35	3	3,3',4	166	6	2,3,4,4',5,6
37	3	3,4,4'	181	7	2,2',3,4,4',5,6
			190	7	2,3,3',4,4',5,6

Analysis of PBDEs in environmental samples

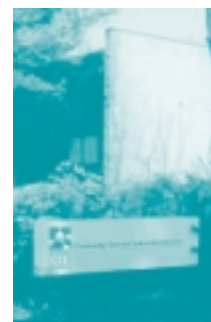
The general procedure for analysis of PBDEs includes extraction and lipid weight determination. Lipids are preferably removed from the extract by partitioning between n-hexane and concentrated sulfuric acid, or by gel permeation chromatography. Further cleanup of the samples may be performed on a small silica gel/sulfuric acid column. Analysis using gas chromatography/mass spectrometry (GC/MS) may be performed using the negative ions formed by electron capture reactions at chemical ionization (ECNI), scanning for m/z 79/81, representing the bromine ion. If gas chromatography with electron capture detector (GC/ECD) is used, it is necessary to remove the more abundant polychlorinated biphenyls that otherwise would interfere with the analyte.

Acknowledgment

The work on PBDEs has been supported by the Swedish EPA, EU (Environment and Climate Program for Research). All references are cited in the complete Applications Note.

Call for user-authored application notes.

The full Applications Note describing the characterization and analysis of PBDEs can be obtained from CIL by requesting Application Note ENV-10. CIL would like to take this opportunity to solicit submissions of additional Applications Notes, which will be cited in The Standard and made available for distribution to any CIL customers who request them. Applications Notes can describe new methods, method improvements, solutions for difficult problems, or broad application areas. Notes may be 1, 2 or 4 pages in length, including figures, tables, and references. Please submit any prospective Applications Note via email to cilmk-tg@isotope.com or to the Marketing Department via fax at 978-749-2768.



New Flame Retardants

CATALOG#	COMPOUND (Isotope, Atom % Enrichment)	SIZE	PRICE
CLM-4694-1.2	Tetrabromobisphenol A (ring- ¹³ C ₁₂ , 99%)	1.2ml	
EO-4930	3,3',4,4',5-Pentabromodiphenyl ether (ring ¹³ C ₁₂ , 99%)	1.2ml	
EO-4915	4-Monobromodiphenyl ether (unlabeled)	1.2ml	
EO-4916	3,3'-Dibromodiphenyl ether (unlabeled)	1.2ml	
EO-4919	2,2',4-Tribromodiphenyl ether (unlabeled)	1.2ml	
EO-4917	2,3',4-Tribromodiphenyl ether (unlabeled)	1.2ml	
EO-4920	2,4,4'-Tribromodiphenyl ether (unlabeled)	1.2ml	
EO-4918	2,2',4,5'-Tetrabromodiphenyl ether (unlabeled)	1.2ml	
EO-4194	2,2',4,4',6-Pentabromodiphenyl ether (unlabeled)	1.2ml	
EO-4921	2,3,4,5,6-Pentabromodiphenyl ether (unlabeled)	1.2ml	
EO-4922	2,2',3,4,4',5'-Hexabromodiphenyl ether (unlabeled)	1.2ml	
EO-4925	2,2',4,4',5,6'-Hexabromodiphenyl ether (unlabeled)	1.2ml	
EO-4923	2,2',3,4,4',6'-Hexabromodiphenyl ether (unlabeled)	1.2ml	
EO-4926	2,2',4,4',6,6'-Hexabromodiphenyl ether (unlabeled)	1.2ml	
EO-4924	2,3,4,4',5,6-Hexabromodiphenyl ether (unlabeled)	1.2ml	
EO-4927	2,2',3,4,4',5,6-Heptabromodiphenyl ether (unlabeled)	1.2ml	

All solutions are offered as 50±5µg/ml in nonane.

New, Suspected Endocrine Disrupting Compounds

Demand for the analysis of suspected endocrine disrupting compounds (EDCs) is one of the fastest growing areas of environmental analysis. Habitats, including soil, sediment, water and air, as well as human and animal exposure, are areas of interest for analysts. CIL's product offerings are expanding. Look for our line of uniformly ¹³C labeled organochlorine pesticides such as Dieldrin (¹³C₁₂, 99%), trans-Nonachlor (¹³C₁₀, 99%) and Oxychlorane (¹³C₁₀, 99%) beginning this summer.

CATALOG#	COMPOUND (Isotope, Atom % Enrichment)	SIZE	PRICE
CLM-4668-1.2	Di-n-Pentyl Phthalate (ring-1,2- ¹³ C ₂ , dicarboxyl- ¹³ C ₂ , 99%)	1.2ml	
CLM-4669-1.2	Di-n-Hexyl Phthalate (ring-1,2- ¹³ C ₂ , dicarboxyl- ¹³ C ₂ , 99%)	1.2ml	
CLM-4670-1.2	Dicyclohexyl Phthalate (ring-1,2- ¹³ C ₂ , dicarboxyl- ¹³ C ₂ , 99%)	1.2ml	
CLM-4671-1.2	Di-n-Propyl Phthalate (ring-1,2- ¹³ C ₂ , dicarboxyl- ¹³ C ₂ , 99%)	1.2ml	
CLM-4674-1.2	n-Butylbenzene (ring- ¹³ C ₆ , 99%)	1.2ml	
CLM-4675-1.2	Bis-(2-Ethylhexyl) Adipate (adipate- ¹³ C ₆ , 99%)	1.2ml	
CLM-4682-1.2	Carbaryl (ring- ¹³ C ₆ , 99%)	1.2ml	
CLM-4683-1.2	Methoxychlor (ring- ¹³ C ₁₂ , 99%)	1.2ml	
CLM-4549-1.2	Permethrin (cis/trans mix)(phenoxy- ¹³ C ₆ , 99%)	1.2ml	
CLM-4551-1.2	2,4,5-Trichlorophenoxyacetic Acid (ring- ¹³ C ₆ , 99%) (in methylene chloride)	1.2ml	

All solutions are offered as 100±µg/ml in nonane unless otherwise noted.

New ¹³C-Labeled Dioxins & Furans

CATALOG#	COMPOUND (Isotope, Atom % Enrichment)	SIZE	PRICE
ED-4169	2-MCDD (¹³ C ₁₂ , 99%)	1.2ml	
ED-4170	2,3-DCDD (¹³ C ₁₂ , 99%)	1.2ml	
EF-4168	2-MCDF (¹³ C ₁₂ , 99%)	1.2ml	
EF-4171	2,4-DCDF (¹³ C ₁₂ , 99%)	1.2ml	
EF-4172	2,4,8-TriCDF (¹³ C ₁₂ , 99%)	1.2ml	
ED-4198	1,3,6,8-TCDD (¹³ C ₁₂ , 99%)	1.2ml	

All solutions are offered as 50±5µg/ml in nonane.



PAH Update New products and reduced prices

As analysts have become more experienced with the analysis of PAHs, they have become convinced that certain aspects of PAH analysis are difficult to perform using deuterated standards because of problems like proton back-exchange during acidic extractions and in the presence of catalytic matrices. This has been documented before, but since PAH analysis has grown to unprecedented levels, the problems are more predominant.

While it is generally agreed that ¹³C PAHs enable superior data quality, because of the high synthetic costs, the price for ¹³C PAHs has in the past been significantly higher than for deuterated PAHs. In an attempt to make these very useful standards more accessible, CIL will offer **¹³C PAH products at 33% off catalog prices** and **¹³C PAH Cocktails at 50% off catalog price** from now until December 31, 1999.

For those who are able to use deuterated PAH standards, but don't want to prepare solutions or deal with excess material, CIL has introduced a line of deuterated PAH solutions, formulated at 200±20µg/ml in isooctane (unless specified otherwise). These handy solutions are only \$95 each. When ten or more are purchased at the same time, the price will be \$47.50 each.

CATALOG#	COMPOUND	CATALOG#	COMPOUND
DLM-108-1.2	Acenaphthene (D ₁₀ , 99%)	DLM-677-1.2	Dibenz[<i>a,h</i>]anthracene (D ₁₄ , 97%)
DLM-2204-1.2	Acenaphthylene (D ₈ , 98%)	DLM-2140-1.2	Fluoranthene (D ₁₀ , 98%)
DLM-102-1.2	Anthracene (D ₁₀ , 98%)	DLM-1123-1.2	Fluorene (D ₁₀ , 98%)
DLM-610-1.2	Benz[<i>a</i>]anthracene (D ₁₂ , 98%)	DLM-2148-1.2	Indeno[1,2,3- <i>c,d</i>]pyrene (D ₁₂ , 98%)
DLM-2136-1.2	Benzo[<i>b</i>]fluoranthene (D ₁₂ , 98%)	DLM-1322-1.2	2-Methylnaphthalene (D ₁₀ , 98%)
DLM-1923-1.2	Benzo[<i>k</i>]fluoranthene (D ₁₂ , 98%)	DLM-365-1.2	Naphthalene (D ₈ , 99%)
DLM-2135-1.2	Benzo[<i>g,h,i</i>]perylene (D ₁₂ , 98%)	DLM-366-1.2	Perylene (in toluene) (D ₁₂ , 98%)
DLM-258-1.2	Benzo[<i>a</i>]pyrene (D ₁₂ , 98%)	DLM-371-1.2	Phenanthrene (D ₁₀ , 98%)
DLM-257-1.2	Benzo[<i>e</i>]pyrene (D ₁₂ , 98%)	DLM-155-1.2	Pyrene (D ₁₀ , 98%)
DLM-261-1.2	Chrysene (in toluene)(D ₁₂ , 98%)		

Finally, to expand our substituted PAH product line, CIL offers the following **new substituted PAH's**.

CATALOG#	COMPOUND	SIZE	PRICE
Nitro-PAHs			
DLM-3836-1.2	5-Nitroacenaphthene (D ₉ , 98%)	1.2ml	
DLM-4712-1.2	9-Nitroanthracene (D ₉ , 98%)	1.2ml	
DLM-4711-1.2	3-Nitrofluoranthene (D ₉ , 98%)	1.2ml	
Alkyl-PAHs			
DLM-2845-1.2	9,10-Dimethylantracene (D ₁₄ , 98%)	1.2ml	
DLM-3840-1.2	7,12-Dimethylbenz[<i>a</i>]anthracene (D ₁₆ , 97%) (in methylene chloride)	1.2ml	
DLM-2852-1.2	1,6-Dimethylnaphthalene (D ₁₂ , 98%)	1.2ml	
DLM-2854-1.2	1,8-Dimethylnaphthalene (D ₁₂ , 98%)	1.2ml	
DLM-2853-1.2	2,6-Dimethylnaphthalene (D ₁₂ , 98%)	1.2ml	
DLM-3842-1.2	5-Methylchrysene (methyl-D ₃ , 98%)	1.2ml	

All solutions are offered as 50±5µg/ml in toluene, unless otherwise noted.

New Pesticides & Metabolites			
CLM-4692-1.2	2,4'-DDT (ring- ¹³ C ₁₂ , 99%)	1.2ml	
CLM-4693-1.2	2,4'-DDE (ring- ¹³ C ₁₂ , 99%)	1.2ml	
DLM-4667-1.2	Phosmet (Dimethyl-D ₆ , 98%)	1.2ml	
CLM-4545-1.2	Fonofos (ring- ¹³ C ₆ , 99%)	1.2ml	
CLM-4542-1.2	3-Phenoxybenzoic acid (phenoxy- ¹³ C ₆ , 99%) (Permethrin metabolite)	1.2ml	
CNLM-4666-1.2	Glyphosate (2- ¹³ C, 99%; ¹⁵ N, 98%)	1.2ml	

All solutions are offered as 100±10µg/ml in nonane, unless otherwise noted.

Additional New Products	
CLM-4567	Thiophenol (¹³ C ₆ , 99%)
CLM-4635	Quinoline (¹³ C ₉ , 99%)

New ¹³C PCBs

As interest in PCB analysis continues to grow, CIL has produced the following new ¹³C PCBs, as well as new PCB formulations.

New Labeled PCBs				
CATALOG#	COMPOUND(Isotope, Atom % Enrichment)	PCB#	SIZE	PRICE
EC-4163	2,4',6-TriCB (¹³ C ₁₂ , 99%)	PCB-32	3ml	
EC-4929	2,2',3,4,4'-PentaCB (¹³ C ₁₂ , 99%)	PCB-85	3ml	
EC-4902	2,3,4,4',5-PentaCB (¹³ C ₁₂ , 99%)	PCB-114	3ml	
EC-4904	2',3,4,4',5-PentaCB (¹³ C ₁₂ , 99%)	PCB-123	3ml	
EC-4167	2,2',4,4',6,6'-HexaCB (¹³ C ₁₂ , 99%)	PCB-155	3ml	
EC-4199	2,3,3',4,4',5,5'-OctaCB (¹³ C ₁₂ , 99%)	PCB-205	3ml	

All solutions are offered as 40±4µg/ml in nonane.

New PCB Formulations				
EC-4187	¹³ C-Labeled Coplanar PCB Mix: 77/81/126/169		3ml	
EC-4189	¹³ C-Labeled Mono-/Deca-PCB Mix: 3/15/28/52/118/153/180/194/208/209		3ml	

CIL also welcomes requests for quotations for custom formulations of ¹³C-PCBs, Native PCBs, and mixtures containing both ¹³C and Native PCBs.



Dioxins and Furans in Polar Solvents

Researchers can now :

- avoid exposure to milligram quantities of potentially harmful chemicals
- decrease disposal costs
- use solutions designed to reduce serial dilution errors

Because of low solubility in methanol, several of these solutions are at concentrations less than the 50µg/ml solutions typically offered by CIL/Radian.

CATALOG#	COMPOUND (Isotope, Atom % Enrichment)	SIZE(concentration)	PRICE
ED-901-A	2,3,7,8-TCDD in Methanol	1.2ml 10µg/ml	
ED-901-B	2,3,7,8-TCDD in DMSO	1.0ml 50µg/ml	
ED-915-M	1,2,7,8-TCDD in Methanol	1.2ml 50µg/ml	
ED-916-M	1,2,8,9-TCDD in Methanol	1.2ml 50µg/ml	
ED-950-M	1,2,3,7,8-PCDD in Methanol	1.2ml 50µg/ml	
ED-960-M	1,2,3,6,7,8-HxCDD in Methanol	1.2ml 1µg/ml	
ED-961-M	1,2,3,4,7,8-HxCDD in Methanol	1.2ml 5µg/ml	
ED-969-M	1,2,3,6,7,8-HxCDD in Methanol	1.2ml 10µg/ml	
EF-903-M	2,3,7,8-TCDF in Methanol	1.2ml 50µg/ml	
EF-918-M	1,2,7,8-TCDF in Methanol	1.2ml 50µg/ml	
EF-953-M	1,2,3,7,8-PCDF in Methanol	1.2ml 50µg/ml	
EF-956-M	2,3,4,7,8-PCDF in Methanol	1.2ml 50µg/ml	
EF-964-M	1,2,3,4,7,8-HxCDF in Methanol	1.2ml 25µg/ml	
EF-962-M	1,2,3,6,7,8-HxCDF in Methanol	1.2ml 10µg/ml	
EF-967-M	1,2,3,7,8,9-HxCDF in Methanol	1.2ml 25µg/ml	
EF-968-M	2,3,4,6,7,8-HxCDF in Methanol	1.2ml 10µg/ml	
EF-973-M	1,2,3,4,6,7,8-HpCDF in Methanol	1.2ml 10µg/ml	

**SPECIAL
OFFER**

Over the years, CIL has introduced numerous new products that are used on a daily basis throughout the world while others have seen more sporadic use. In some cases, special cocktails were made that were never included in the catalog or publicized elsewhere.

Now is your opportunity to acquire some of these materials. Over the summer months, you will receive this listing of products. If you do not receive a copy you may request one via email at cilsales@isotope.com.



Nitrosamine Solutions

OSHA regulations described in 29CFR §1910.1003 and parts following prohibit handling and storage of N-Nitrosodimethylamine at concentrations greater than 1% (10mg/ml or 10mg/gm, whichever is higher) in most laboratories. CIL takes the risk away from you, and enables you to comply with OSHA regulations by offering solutions of several nitrosamines at concentrations of 1mg/ml.

- NLM-3432-S N-Nitrosodiethylamine (¹⁵N₂, 99%) @ 1mg/ml in CD₂Cl₂
- DLM-2130-S N-Nitrosodimethylamine (D₆, 98%) @ 1mg/ml in CD₂Cl₂
- DLM-2131-S N-Nitrosodi-n-propylamine (D₁₄, 98%) @ 1mg/ml in CD₂Cl₂
- DLM-3098-S N-Nitrosodiphenylamine (2,2',4,4',6,6'-D₆, 98%) @ 1mg/ml in CD₂Cl₂

CIL offers many of its products, both hazardous and less hazardous, in convenient quantitative solutions in just the amounts you need for your analysis. Reduce exposure during standards preparation and internal QC expenditures, and reduce costly disposal of excess neat material by using CIL's quantitative standards.

Lake Apopka Pelican Pesticide Poisoning

While at PittCon '99 in Orlando, Florida during the first week of March, we received another reminder of the longevity of Persistent Organic Pollutants (POPs). The large lake nearest to Orlando, Lake Apopka, had received attention in recent years when one of the local endocrinologists, Dr. Louis Guillette of the University of Florida, started to assess the effect of pollutants on local species by measuring the developmental abnormalities of the reproductive systems of alligators. Lake Apopka had been subjected over the years to a substantial amount of agricultural runoff, and there was concern that it was affecting the reproductive systems of wildlife and perhaps humans. Concurrently, there were plans to return some of the drained swamplands surrounding Lake Apopka, which had been converted to agricultural use, back to their original role as wetlands. Unfortunately, it appears that as the fields filled with

water, pesticides, including Dieldrin, DDT and its metabolites, and other harmful chemicals began leaching out of the soil, killing hundreds of pelicans and other wildlife.



New Pesticide Metabolites Initiative

You may have noticed a recent surge of Pesticide Metabolites listed in The Standard. For example, CIL is offering 4-Nitrophenol (CLM-789) as the metabolite of Methyl Parathion; 3-Phenoxybenzoic acid (CLM-4550-1.2) as the metabolite of Permethrin; Oxypyrimidine (2-Isopropyl-6-methyl-4-pyridinol; CLM-4538-1.2) as the metabolite of Diazinon. Many customers look at pesticides after they have entered into humans or animals, or after weathering has occurred. Metabolites contribute additional information about the overall burden of a pesticide on a biological or environmental system. A full cross-reference of Metabolites and Parent Pesticides can be obtained by requesting Applications Note ENV-11. User additions are welcome. Please let us know if there are labeled pesticide metabolites you would like to see CIL offer. Send your requests to Terry Grim via fax at 978-749-2768, or via e-mail at terryg@isotope.com.

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