

# PBDE Metabolites



## Hydroxy and Methoxy Polybromodiphenyl Ether Congeners

Hydroxylated and methoxylated PBDEs may be formed as metabolites of the PBDE flame retardants. Hydroxylated PBDEs (OH-PBDEs) have been detected in human blood, mice, rats, fish and birds. They have been studied for their potential to disrupt the endocrine (hormone) system in mammals. One important aspect of these studies is the structural similarity of some of the OH-PBDEs with the **thyroid hormones** which affect every cell in the body. At AccuStandard we have synthesized a variety of hydroxylated and methoxylated PBDEs. HBDE-3007 (**T2-like**), HBDE-4010 (**T3-like**), and HBDE-5010 (**T4-like**) display the closest similarity to the halogen substitution pattern of those thyroid hormones.

AccuStandard recognizes the significance of this on-going research and is supporting it by providing the necessary reference standards. Please check the website for the latest update of synthesized OH- and MeO-PBDEs, or request specific congeners to be synthesized.

Short Form	Compound	Conc.	Solvent	Cat. No.	1 mL
<b>Hydroxy</b>					
2'-OH-BDE-003	2'-Hydroxy-4-monobromodiphenyl ether	50 µg/mL	AcCN	HBDE-1001S-CN	
3'-OH-BDE-007	3'-Hydroxy-2,4-dibromodiphenyl ether	50 µg/mL	AcCN	HBDE-2001S-CN	
2'-OH-BDE-007	2'-Hydroxy-2,4-dibromodiphenyl ether	10 µg/mL	AcCN	HBDE-2002S-CN-0.2X	
2'-OH-BDE-009	2'-Hydroxy-2,5-dibromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-2003S-CN	
4'-OH-BDE-017	4'-Hydroxy-2,2',4-tribromodiphenyl ether	50 µg/mL	AcCN	HBDE-3001S-CN	
3'-OH-BDE-028	3'-Hydroxy-2,4,4'-tribromodiphenyl ether	50 µg/mL	AcCN	HBDE-3002S-CN	
2'-OH-BDE-028	2'-Hydroxy-2,4,4'-tribromodiphenyl ether	50 µg/mL	AcCN	HBDE-3003S-CN	
5'-OH-BDE-025	5'-Hydroxy-2,3',4-tribromodiphenyl ether	50 µg/mL	AcCN	HBDE-3004S-CN	
3'-OH-BDE-029	3'-Hydroxy-2,4,5-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-3005S-CN	
3'-OH-BDE-030	3'-Hydroxy-2,4,6-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-3006S-CN	
4'-OH-BDE-030	4'-Hydroxy-2,4,6-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-3007S-CN	
4-OH-BDE-042	4-Hydroxy-2,2',3,4'-tetrabromodiphenyl ether	10 µg/mL	AcCN	HBDE-4001S-CN-0.2X	
4'-OH-BDE-049	4'-Hydroxy-2,2',4,5'-tetrabromodiphenyl ether	10 µg/mL	AcCN	HBDE-4002S-CN-0.2X	
3-OH-BDE-047	3-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	50 µg/mL	AcCN	HBDE-4003S-CN	
5-OH-BDE-047	5-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	50 µg/mL	AcCN	HBDE-4004S-CN	
6-OH-BDE-047	6-Hydroxy-2,2',4,4'-tetrabromodiphenyl ether	10 µg/mL	AcCN	HBDE-4005S-CN-0.2X	
		10 µg/mL	Toluene	HBDE-4005S-T-0.2X	
2'-OH-BDE-068	2'-Hydroxy-2,3',4,5'-tetrabromodiphenyl ether	10 µg/mL	AcCN	HBDE-4006S-CN-0.2X	
		10 µg/mL	Toluene	HBDE-4006S-T-0.2X	
		50 µg/mL	AcCN	HBDE-4006S-CN	
		50 µg/mL	Toluene	HBDE-4006S-T	
6'-OH-BDE-066	6'-Hydroxy-2,3',4,4'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-4008S-CN	
5'-OH-BDE-069	5'-Hydroxy-2,3',4,6'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-4009S-CN	
4'-OH-BDE-069	4'-Hydroxy-2,3',4,6'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-4010S-CN	
4'-OH-BDE-048	4'-Hydroxy-2,2',4,5'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-4011S-CN	
4-OH-BDE-090	4-Hydroxy-2,2',3,4',5'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5001S-CN-0.2X	
6-OH-BDE-085	6-Hydroxy-2,2',3,4,4'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5002S-CN-0.2X	
6-OH-BDE-087	6-Hydroxy-2,2',3,4,5'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5003S-CN-0.2X	
5'-OH-BDE-100	5'-Hydroxy-2,2',4,4',6'-pentabromodiphenyl ether <b>NEW</b>	10 µg/mL	AcCN	HBDE-5004S-CN-0.2X	
6-OH-BDE-082	6-Hydroxy-2,2',3,3',4'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5005S-CN-0.2X	
6'-OH-BDE-099	6'-Hydroxy-2,2',4,4',5'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5006S-CN-0.2X	
5'-OH-BDE-099	5'-Hydroxy-2,2',4,4',5'-pentabromodiphenyl ether	10 µg/mL	AcCN	HBDE-5007S-CN-0.2X	
3-OH-BDE-100	3-Hydroxy-2,2',4,4',6'-pentabromodiphenyl ether	50 µg/mL	AcCN	HBDE-5008S-CN	
4'-OH-BDE-101	4'-Hydroxy-2,2',4,5,5'-pentabromodiphenyl ether	50 µg/mL	AcCN	HBDE-5009S-CN	
4'-OH-BDE-121	4'-Hydroxy-2,3',4,5',6'-pentabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-5010S-CN	
6-OH-BDE-123	6-Hydroxy-2',3,4,4',5'-pentabromodiphenyl ether <b>NEW</b>	50 µg/mL	AcCN	HBDE-5011S-CN	
6-OH-BDE-157	6-Hydroxy-2,3,3',4,4',5'-hexabromodiphenyl ether	10 µg/mL	AcCN	HBDE-6001S-CN-0.2X	
6-OH-BDE-140	6-Hydroxy-2,2',3,4,4',6'-hexabromodiphenyl ether	10 µg/mL	AcCN	HBDE-6002S-CN-0.2X	
3'-OH-BDE-154	3'-Hydroxy-2,2',4,4',5,6'-hexabromodiphenyl ether	10 µg/mL	AcCN	HBDE-6003S-CN-0.2X	
6-OH-BDE-137	6-Hydroxy-2,2',3,4,4',5'-hexabromodiphenyl ether	10 µg/mL	AcCN	HBDE-6004S-CN-0.2X	
3-OH-BDE-155	3-Hydroxy-2,2'-4,4',6',6'-hexabromodiphenyl ether <b>NEW</b>	10 µg/mL	AcCN	HBDE-6005S-CN-0.2X	
		50 µg/mL	AcCN	HBDE-6005S-CN	
4-OH-BDE-146	4-Hydroxy-2,2',3,4,4',5,5'-hexabromodiphenyl ether <b>NEW</b>	10 µg/mL	AcCN	HBDE-6006S-CN-0.2X	
		50 µg/mL	Isooctane	HBDE-6006S	
4-OH-BDE-187	4-Hydroxy-2,2',3,4',5,5',6'-heptabromodiphenyl ether	50 µg/mL	AcCN	HBDE-7001S-CN	
6-OH-BDE-180	6-Hydroxy-2,2',3,4,4',5,5'-heptabromodiphenyl ether	50 µg/mL	AcCN	HBDE-7002S-CN	
4-OH-BDE-188	4-Hydroxy-2,2',3,4',5,6,6'-heptabromodiphenyl ether	50 µg/mL	AcCN	HBDE-7003S-CN	
6-OH-BDE-182	6-Hydroxy-2,2',3,4,4',5,6'-heptabromodiphenyl ether	50 µg/mL	AcCN	HBDE-7004S-CN-0.2X	
4'-OH-BDE-201	4'-Hydroxy-2,2',3,3',4,5',6,6'-octabromodiphenyl ether	50 µg/mL	AcCN	HBDE-8001S-CN	

Methoxy PBDE Congeners  
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# PBDE Metabolites

## Methoxy Polybromodiphenyl Ether Congeners

Short Form	Compound	Conc.	Solvent	Cat. No.	1 mL
<b>Methoxy</b>					
2'-MeO-BDE-003	2'-Methoxy-4-monobromodiphenyl ether	50 µg/mL	MeOH	MOBDE-1001S	
3'-MeO-BDE-007	3'-Methoxy-2,4-dibromodiphenyl ether	50 µg/mL	MeOH	MOBDE-2001S	
2'-MeO-BDE-007	2'-Methoxy-2,4-dibromodiphenyl ether	10 µg/mL	MeOH	MOBDE-2002S-0.2X	
2'-MeO-BDE-009	2'-Methoxy-2,5-dibromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-2003S	
4'-MeO-BDE-017	4'-Methoxy-2,2',4-tribromodiphenyl ether	50 µg/mL	MeOH	MOBDE-3001S	
3'-MeO-BDE-028	3'-Methoxy-2,4,4'-tribromodiphenyl ether	50 µg/mL	MeOH	MOBDE-3002S	
2'-MeO-BDE-028	2'-Methoxy-2,4,4'-tribromodiphenyl ether	50 µg/mL	MeOH	MOBDE-3003S	
5'-MeO-BDE-025	5'-Methoxy-2,3',4-tribromodiphenyl ether	50 µg/mL	MeOH	MOBDE-3004S	
3'-MeO-BDE-029	3'-Methoxy-2,4,5-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-3005S	
3'-MeO-BDE-030	3'-Methoxy-2,4,6-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-3006S	
4'-MeO-BDE-030	4'-Methoxy-2,4,6-tribromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-3007S	
4-MeO-BDE-042	4-Methoxy-2,2',3,4'-tetrabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-4001S-0.2X	
4'-MeO-BDE-049	4'-Methoxy-2,2',4,5'-tetrabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-4002S-0.2X	
3-MeO-BDE-047	3-Methoxy-2,2',4,4'-tetrabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-4003S	
5-MeO-BDE-047	5-Methoxy-2,2',4,4'-tetrabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-4004S	
6-MeO-BDE-047	6-Methoxy-2,2',4,4'-tetrabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-4005S-0.2X	
2'-MeO-BDE-068	2'-Methoxy-2,3',4,5'-tetrabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-4006S-0.2X	
2'-MeO-BDE-075	2'-Methoxy-2,4,4',6'-tetrabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-4007S	
6'-MeO-BDE-066	6'-Methoxy-2,3',4,4'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-4008S	
5'-MeO-BDE-069	5'-Methoxy-2,3',4,6'-tetrabromodiphenyl ether <b>NEW</b>	10 µg/mL	MeOH	MOBDE-4009S-0.2X	
		50 µg/mL	MeOH	MOBDE-4009S	
4'-MeO-BDE-069	4'-Methoxy-2,3',4,6'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-4010S	
4'-MeO-BDE-048	4'-Methoxy-2,2',4,5'-tetrabromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-4011S	
4-MeO-BDE-090	4-Methoxy-2,2',3,4',5'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5001S-0.2X	
6-MeO-BDE-085	6-Methoxy-2,2',3,4,4'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5002S-0.2X	
6-MeO-BDE-087	6-Methoxy-2,2',3,4,5'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5003S-0.2X	
5'-MeO-BDE-100	5'-Methoxy-2,2',4,4',6'-pentabromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-5004S	
6-MeO-BDE-082	6-Methoxy-2,2',3,4,3',4'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5005S-0.2X	
6'-MeO-BDE-099	6'-Methoxy-2,2',4,4',5'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5006S-0.2X	
5'-MeO-BDE-099	5'-Methoxy-2,2',4,4',5'-pentabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-5007S-0.2X	
3-MeO-BDE-100	3-Methoxy-2,2',3,4,4',6'-pentabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-5008S	
4'-MeO-BDE-101	4'-Methoxy-2,2',4,5,5'-pentabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-5009S	
4'-MeO-BDE-121	4'-Methoxy-2,3',4,5',6'-pentabromodiphenyl ether <b>NEW</b>	50 µg/mL	MeOH	MOBDE-5010S	
6-MeO-BDE-123	6-Methoxy-2',3,4,4',5'-pentabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-5011S	
6-MeO-BDE-157	6-Methoxy-2,3,3',4,4',5'-hexabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-6001S-0.2X	
6-MeO-BDE-140	6-Methoxy-2,2',3,4,4',6'-hexabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-6002S-0.2X	
3'-MeO-BDE-154	3'-Methoxy-2,2',4,4',5,6'-hexabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-6003S-0.2X	
6-MeO-BDE-137	6-Methoxy-2,2',3,4,4',5'-hexabromodiphenyl ether <b>NEW</b>	10 µg/mL	MeOH	MOBDE-6004S-0.2X	
3-MeO-BDE-155	3-Methoxy-2,2',4,4',6,6'-hexabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-6005S-0.2X	
		50 µg/mL	MeOH	MOBDE-6005S	
4-MeO-BDE-146	4-Methoxy-2,2',3,4',5,5'-hexabromodiphenyl ether <b>NEW</b>	10 µg/mL	MeOH	MOBDE-6006S-0.2X	
4-MeO-BDE-187	4-Methoxy-2,2',3,4',5,5',6'-heptabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-7001S	
6-MeO-BDE-180	6-Methoxy-2,2',3,4,4',5,5'-heptabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-7002S	
4-MeO-BDE-188	4-Methoxy-2,2',3,4',5,6,6'-heptabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-7003S	
6-MeO-BDE-182	6-Methoxy-2,2',3,4,4',5,6'-heptabromodiphenyl ether	10 µg/mL	MeOH	MOBDE-7004S-0.2X	
4'-MeO-BDE-201	4'-Methoxy-2,2',3,3',4,5',6,6'-octabromodiphenyl ether	50 µg/mL	MeOH	MOBDE-8001S	

## Mixed Bromo/Chloro Hydroxylated Diphenyl Ethers



The abundance of PBDEs in the environment led to the increased detection of hydroxylated PBDEs (OH-PBDEs) as well as their chlorinated derivatives (OH-PBCDEs) especially in aquatic environments. Several pathways of their formation have been described in the literature.

In saltwater systems, some of the OH-PBDEs are being produced naturally; while in freshwater systems, atmospheric and wastewater treatment oxidation seems to be the major source of these compounds. Furthermore, disinfection of wastewater with chlorine may lead to the chlorination of OH-PBDEs. These mixed bromo/chloro hydroxy diphenyl ethers (OH-PBCDEs) can then undergo photochemical cyclization in the presence of sunlight to form the potentially even more harmful brominated/chlorinated dibenzo-p-dioxins (Br/Cl-DDs). There is growing concern that both naturally and anthropogenically produced PBDDs and Br/Cl-DDs are an emerging environmental problem.

At AccuStandard, following the lead of environmental chemists, we recognize the emerging problem of the presence of OH-PBCDEs. We have synthesized three OH-PBCDEs and their methylated counterparts to provide reference standards for this new group of compounds. All three chlorinated OH-PBDEs are based on the structure of BDE-47, the most common BDE congener found in environmental samples.

AccuStandard will synthesize more derivatives as demand for these compounds develops.

Compound (Short Form)	Conc.	Solvent	Cat. No.	1 mL
<b>Hydroxy</b>				
3-Chloro-6-hydroxy-2,2',4,4'-tetrabromodiphenyl ether (3-Cl-6-OH-BDE-047)	25 µg/mL	Acetonitrile	HCBDE-4001S-0.5X	
	50 µg/mL	Acetonitrile	HCBDE-4001S	
3,5-Dichloro-6-hydroxy-2,2',4,4'-tetrabromodiphenyl ether (3,5-Cl <sub>2</sub> -6-OH-BDE-047)	25 µg/mL	Acetonitrile	HCBDE-4002S-0.5X	
	50 µg/mL	Acetonitrile	HCBDE-4002S	
5-Chloro-6-hydroxy-2,2',4,4'-tetrabromodiphenyl ether (5-Cl-6-OH-BDE-047)	25 µg/mL	Acetonitrile	HCBDE-4003S-0.5X	
	50 µg/mL	Acetonitrile	HCBDE-4003S	
<b>Methoxy</b>				
3-Chloro-6-methoxy-2,2',4,4'-tetrabromodiphenyl ether (3-Cl-6-MeO-BDE-047)	25 µg/mL	Methanol	MOCBDE-4001S-0.5X	
	50 µg/mL	Methanol	MOCBDE-4001S	
3,5-Dichloro-6-methoxy-2,2',4,4'-tetrabromodiphenyl ether (3,5-Cl <sub>2</sub> -6-MeO-BDE-047)	25 µg/mL	Methanol	MOCBDE-4002S-0.5X	
	50 µg/mL	Methanol	MOCBDE-4002S	
5-Chloro-6-methoxy-2,2',4,4'-tetrabromodiphenyl ether (5-Cl-6-MeO-BDE-047)	25 µg/mL	Methanol	MOCBDE-4003S-0.5X	
	50 µg/mL	Methanol	MOCBDE-4003S	