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EPA Great Lakes Study for Identification of PBTs to Develop Analytical Methods: Selection of Additional PBTs, Use, and Potential Environmental Release of Priority Chemicals – Progress Report – February 2009

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I. INTRODUCTION

Of the approximately 600 chemicals that were initially selected as potential PBTs, Derik Muir selected 50 chemicals (10 chemicals from each of the following classes – brominated chemicals, siloxanes, perfluorinated chemicals, chlorinated chemicals, and non-halogenated chemicals). The approximately 600 chemicals included an initial 429 high-production chemicals and another approximately 180 mid- and low-production chemicals as well as potential biomagnifiers in air breathing organisms. The major criteria used to select the top 10 were production volume, bioconcentration factor (BCF), and persistence (AO $t_{1/2}$). We also sought to identify representatives of important classes of compounds such as TBBPA derivatives, cyclic siloxanes, chlorinated pyridines, and cyclopentane/enes. We omitted most chemicals for which there were already measurements (e.g., PBDEs, synthetic musks, triaryl phosphates, haloalkyl phosphates), although some were included to provide reference points for the new ones selected.

For the July 17, 2008 GLBTS Surveillance meeting at the Canadian Center for Inland Waters, it was agreed that these top 50 would be reviewed for use and potential release in order to select chemicals for the monitoring programs. It was further decided that although the siloxane chemicals were still of interest, that the analytical capabilities were such that they should not be considered for this meeting. In that meeting, the use and environmental release as well as any other relevant information for the 40 chemicals (siloxanes excluded) were presented to focus on good new PBT candidates.

Since that July meeting, SRC has focused on two activities: (1) getting the Inventory Update Rule production data for 2006 and adding it to our database; and (2) evaluating the use/release information on the 59 brominated chemicals that were non-top 10 priority. Those activities were the focus of our November 2008 progress report. This report focuses on three activities: (1) identification of the chlorinated chemicals to assess their use and potential release; (2) review of the European chemical Substances Information System (ESIS) list of 127 PBT chemicals; and (3) screening of the chemicals unique to the 2006 IUR.

II. IDENTIFICATION OF THE CHLORINATED CHEMICALS

From the 602 potential PBT chemicals originally selected, the 59 priority brominated chemicals were removed (leaving 543 chemicals). A substructure search of the 543 chemicals was conducted using C-Cl to identify 135 chemicals. A search of that file for C-CF₂-C identified 4 chemicals that should be in the fluorochemicals classes leaving 131 chemicals. Also subtracted were 5 chemicals that were organophosphates (although they have some halogens on the alcohol portion) since they would be better characterized in the “Non-Halogenated” PBT category. This left 126 chemicals in the chlorinated chemicals class. Some of these may not be good emerging PBT; for example benzotrichlorides (three chlorides on the benzyl carbon) hydrolyze very rapidly (half-life = 19 seconds; Mabey and Mill, 1978)¹ and therefore, the hydrolysis products will need to be considered. In the next several months, these 126 chemicals will be assessed for use and potential environmental release. Also, three chlorinated chemicals from the ESIS PBT list have been added: 1,2,4-trichlorobenzene, 1,2,3-trichlorobenzene, and hexachlorobutadiene. All three of these have been rated as PBTs by the European Commission and have been detected previously in environmental samples. Therefore, they are added for comparison but are not necessarily good “new” emerging contaminants.

¹ Mabey, W. and Mill, T. (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. J. Phys. Chem. Ref. Data 7(2): 383-409.

III. REVIEW OF THE EUROPEAN CHEMICAL SUBSTANCES INFORMATION SYSTEM (ESIS) LIST OF 127 PBT CHEMICALS

The ESIS list of PBT chemicals are chemicals that are being evaluated by a variety of countries under the Interim Strategy for REACH and the Existing Substances Regulation (ESR) program (Priority Lists, Risk Assessment process and tracking system in relation to Council Regulation (EEC) 793/93, <http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=pbt>).

The overall results of the evaluation from the website are:

Substances fulfilling PBT or vBvP or POP criteria:	27
Substances not fulfilling:	66
Substances under evaluation:	24
Substances deferred:	10
Total:	127

Many of the chemicals are complex mixtures, drugs, and pesticides which are not expected to be in the DSL/IUR database. The first step with the ESIS PBT list was to match the 127 chemicals with the DSL/IUR database – the following 29 ESIS PBT chemicals were not in the DSL/IUR database:

Table 1. ESIS PBT Chemicals Not in DSL/IUR Database (ID# from the PBT database when sorted by CAS#)

ID#	CAS#	Chemical Name	Comment
10	88-06-2	2,4,6-Trichlorophenol	Made mostly in OECD countries; widely used in the synthesis of a fungicide, prochloraz (67747-09-5)
102	84852-14-2	2,4-Dinonylphenol, branched	Ullmann – ethoxylate used as technical emulsifiers; dinonylphenols – not specific isomer in Ullmann or KO; ESIS database – deferred
110	90552-07-1	2-Propenoic acid, 2-methyl-, C ₉ -C ₁₁ -isoalkyl esters, C ₁₀ -rich	No KO or Ullmann; ESIS database not fulfilling PBT criteria; no profile
57	5208-93-5	3-Methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol	No KO or Ullmann; ESIS database – does not met PBT criteria – profile available; two biodegradation studies very close to passing; not P but maybe B
68	14861-17-7	4(2,4-Dichlorophenoxy)aniline	No KO or Ullmann; ESIS database profile; Aminofen, conclusion, may be P but fails OECD301D; log K _{ow} 3.8 – doesn't meet the screening criteria so not a PBT
49	2392-48-5	4-Chloro-1-(2,4-dichlorophenoxy)-2-nitrobenzene	No KO or Ullmann; ESIS database profile, less than 1% in OECD 301B, not B; logK _{ow} is 3.82 – below screening trigger of 4.5
119	91745-46-9	Amines, C ₁₂ -C ₁₄ -alkyl, reaction products with hexanol, phosphorus oxide	P2 – no KO or Ullmann; deferred ESIS database
	120-12-7	Anthracene	In DSL/IUR database; 10-500K in 2002, not reported in 2006
ESIS database had the following chemicals fulfilling PBT criteria based upon assessment for anthracene:			
113	90640-81-6	Anthracene oil, anthracene paste	
121	91995-15-2	Anthracene oil, anthracene paste, anthracene fraction	

Table 1. ESIS PBT Chemicals Not in DSL/IUR Database (ID# from the PBT database when sorted by CAS#)

ID#	CAS#	Chemical Name	Comment
122	91995-17-4	Anthracene oil, anthracene paste, distn. lights	
114	90640-82-7	Anthracene oil, anthracene low	
118	91696-73-0	Benzenesulfonic acid, C ₁₄ -C ₄₄ -branched and linear alkyl derivatives, calciums	No KO or Ullmann; the branched ABS is known to be non-biodegraded; from the 1960's – foaming of rivers; linear – LAS is very biodegradable
85	39489-75-3	Bis(2,4-dichloro-5-nitrophenyl) carbonate	No KO or Ullmann; ESIS database deferred
1	50-29-3	Clofenotane (= p,pDDT):	Insecticide; ESIS database – no profile
80	31565-23-8	Di(tert-dodecyl) pentasulphide	No KO or Ullmann; ESIS database – under evaluation
17	115-32-2	Dicofol	Acaricide similar structure to DDT OH on benzyl C
123	91995-42-5	Distillates (coal tar), heavy oils, pyrene fraction	No KO or Ullmann
124	91995-52-7	Distillates (coal tar), pitch, pyrene fraction	No KO or Ullmann
16	115-29-7	Endosulfan	Broad spectrum insecticide; hydrolysis at sulfite ester bonds
64	11081-15-5	Isooctylphenol	Ullmann – alkylating olefin dibutene; no KO; ESIS database deferred
88	51338-27-3	Methyl 2(4-(2,4-dichlorophenoxy)phenoxy) propionate	KO; herbicide – diclofop, methyl
76	26272-76-4	N[2-(2-Heptadecyl-4,5-dihydro-1H-imidazol-1-yl)ethyl] stearamide	No KO or Ullmann; ESIS database – no profile; does not fulfill PBT
46	1836-75-5	Nitrofen	Herbicide
109	90481-05-3	Phenol, nonyl, manuf. of, by-products from, high-boiling	No KO or Ullmann
125	92061-94-4	Residues (coal tar), pitch distn.	No KO or Ullmann
116	91082-17-6	Sulfonic acids, C ₁₀ -C ₂₁ -alkane, Ph esters	No KO or Ullmann; looks like LAS isomers
63	8052-10-6	Talloil rosin	No KO or Ullmann (name search)
120	91770-80-8	Terpenes and terpenoids, turpentineoil, 3-carene fraction	No KO or Ullmann
108	86089-17-0	Tridecylamine, branched and linear	No KO or Ullmann

This leaves 98 chemicals that were in the ESIS database of PBT chemicals and the DSL/IUR database. The priority 602 PBT chemicals that were selected by us matched up with 27 chemicals from the ESIS database and are listed in Table 2.

Table 2. Twenty-seven PBT Chemicals from the ESIS Database and Priority 602 DSL/IUR

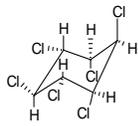
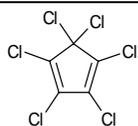
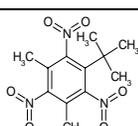
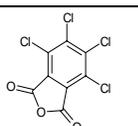
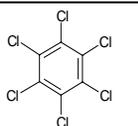
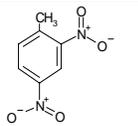
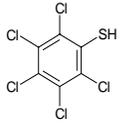
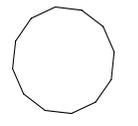
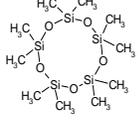
ID	Molstructure	Kowwin	Cus98	Cus02	ESIS Sum	ESIS Con
000058-89-9		4.26	10K - 500K	No Reports		Fulfilling POP criteria
000077-47-4		4.63	>10M - 50M	>10M - 50M		Deferred
000081-15-2		4.45	10K - 500K	10K - 500K		Under evaluation
000117-08-8		4.65	>1M - 10M	>1M - 10M	>view	Not fulfilling PBT & vPvB criteria
000118-74-1		5.86	10K - 500K	10K - 500K		Fulfilling POP criteria
000121-14-2		2.18	>500K - 1M	10K - 500K	>view	Not fulfilling PBT & vPvB criteria
000133-49-3		5.91	10K - 500K	10K - 500K	>view	Fulfilling PBT & vPvB criteria
000294-62-2		6.12	>50M - 100M	>50M - 100M	>view	Fulfilling PBT criteria
000541-02-6		5.71	>50M - 100M	>100M - 500M		Under evaluation

Table 2. Twenty-seven PBT Chemicals from the ESIS Database and Priority 602 DSL/IUR

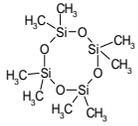
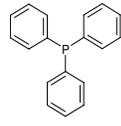
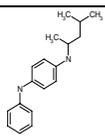
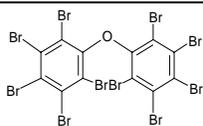
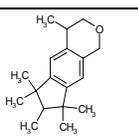
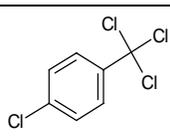
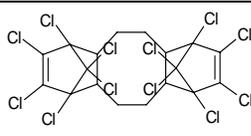
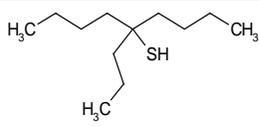
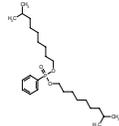
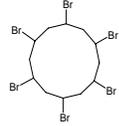
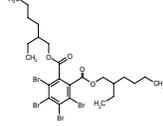
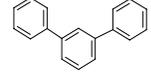
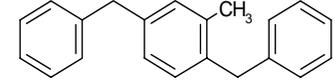
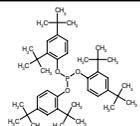
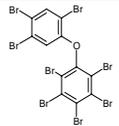
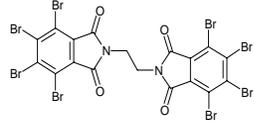
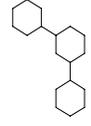
ID	Molstructure	Kowwin	Cus98	Cus02	ESIS Sum	ESIS Con
000556-67-2		5.09	>100 M - 500M	>100M - 500M		Under evaluation
000603-35-0		5.02	>1M - 10M	>1M - 10M	>view	Not fulfilling PBT & vPvB criteria
000608-71-9		5.96				Deferred
000793-24-8		4.68	>50M - 100M	>50M - 100M		Not fulfilling PBT & vPvB criteria
001163-19-5		12.11	>50M - 100M	>50M - 100M		Under evaluation
001222-05-5		6.26	>1M - 10M	>1M - 10M		Not fulfilling PBT & vPvB criteria
005216-25-1		4.54	>10M - 50M	No Reports	>view	Not fulfilling PBT & vPvB criteria
013560-89-9		11.27	>1M - 10M	>1M - 10M		Deferred
025103-58-6		6.07	>10M - 50M	>10M - 50M		Under evaluation

Table 2. Twenty-seven PBT Chemicals from the ESIS Database and Priority 602 DSL/IUR

ID	Molstructure	Kowwin	Cus98	Cus02	ESIS Sum	ESIS Con
025550-98-5		9.32	>1M - 10M	>1M - 10M	>view	Not fulfilling PBT & vPvB criteria
025637-99-4		7.74	10K - 500K	10K - 500K		Fulfilling PBT criteria
026040-51-7		11.95	>1M - 10M	>1M - 10M		Deferred
026140-60-3	 MIXTURE OF DIPHENYL ISOMERS	5.52	>10M - 50M	>10M - 50M		Under evaluation
026898-17-9		6.59	10K - 500K	>500K - 1M	>view	Not fulfilling PBT & vPvB criteria
031570-04-4		18.08	>10M - 50M	>10M - 50M		Under evaluation
032536-52-0		10.33	>1M - 10M	>1M - 10M		Fulfilling PBT criteria
032588-76-4		9.8	>10M - 50M	>1M - 10M	>view	Not fulfilling PBT & vPvB criteria
061788-32-7		8.55	>1M - 10M	>10M - 50M		Under evaluation

These 27 PBT chemicals that overlap between the ESIS PBT list and the 602 DSL/IUR priority PBTs will be discussed in the five chemical groups as the assessment of use and environmental release is conducted. However, a few brief comments on some of them follow. Several of these fall into the brominated chemicals category. Two of them (001163-19-5 and 032536-52-0) are polybrominated diphenyl ethers (PBDEs) which are well known environmental contaminants. Three of the these brominated chemicals are on our priority list – hexabromocyclododecane (HBCD) (025637-99-4), bis-2-ethylhexyl tetrabromophthalate (26040-51-7), and ethylene bis(tetrabromophthalimide) (032588-76-4). As indicated in our November report, HBCD has been detected in environmental media (blubber of porpoises and dolphins and in household dust) and bis-2-ethylhexyl tetrabromophthalate has been recently detected in household dust. However, the European Commission (ESIS database) has concluded that ethylene bis(tetrabromophthalimide) does not fulfill PBT or vPvB criteria and provided a summary fact sheet (have “>view” in Table 2). The summary fact sheet indicates ethylene bis(tetrabromophthalimide) does not biodegrade (MITI OECD 301C test negative), but a narrative suggests that by analogy to other halogenated chemicals, dehalogenation may occur under anaerobic conditions. This still suggests that the chemical will be persistent. The summary fact sheet also suggests that bioaccumulation is not likely because of the high molecular weight, its measured octanol solubility, and its maximum cross-sectional diameter. There was a measured BCF value (MITI test with carp) but the results (BCF <3.3) were considered unusable because the test concentration exceeded the water solubility. Thus, the conclusion of not fulfilling PBT and vPvB is not well supported, and there are examples of chemicals with high molecular weight and K_{ow} (e.g., HBCD and Dechlorane-Plus [13560-89-9 in Table 2]) that have been detected in environmental samples. Therefore, it seems reasonable to leave ethylene bis(tetrabromophthalimide) on the high priority brominated compounds list.

Several compounds in Table 2 are musks that have been detected in the environment (see Howard and Meylan, 2007 report). This includes musk xylene (MX, 81-15-2) and HHCB (1222-05-5). Several of the chlorinated compounds are on the priority list of chlorinated compounds or on the list of 126 chlorinated compounds identified above. These will be discussed during the use and environmental release analysis of the chlorinated compounds.

The remaining 71 chemicals that were listed on the ESIS PBT list and were in the DSL/IUR database, but not in the priority 602 chemicals are listed below:

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

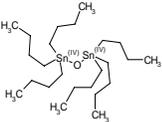
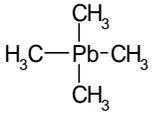
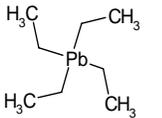
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
000056-35-9		4.05	10K - 500K	10K - 500K	ESIS profile: transforms to tributyl tin which is a PBT
000075-74-1		2.92	No Reports	No Reports	
000078-00-2		4.88	>1M - 10M	>1M - 10M	ESIS Profile: TetraEt hydrolyze rapidly to triethyl lead salt that is not PBT; TEPb does bioconcentrate

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

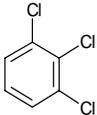
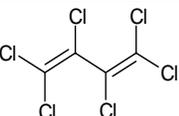
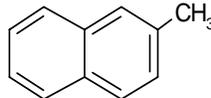
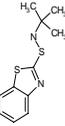
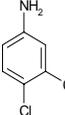
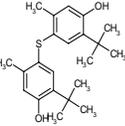
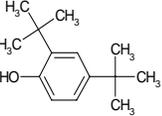
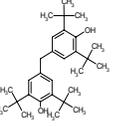
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
000087-61-6		3.93	No Reports	10K - 500K	ESIS profile: 1,2,3-isomer considered PBT by analogy to 1,2,4-isomer; repellents for wood-feeding insects; Ullmann
000087-68-3		4.72	No Reports	10K - 500K	Inadvertent by-product from chlorinated solvent production; Tox Profile available (hexachloro-1,3-butadiene)
000091-57-6		3.72	10K - 500K	No Reports	ESIS profile: P - half-life 350-500 days; B - below 2000
000095-31-8		2.56	>10M - 50M	>10M - 50M	ESIS Profile: not P because of fast hydrolysis (hours)
000095-76-1		2.37	No Reports	No Reports	
000096-69-5		8.24	>500K - 1M	>500K - 1M	
000096-76-4		5.33	>10M - 50M	>50M - 100M	ESIS profile: may be P but its similarity to BHT would suggest it may be biodegradable; not B - experimental in hundreds
000118-82-1		8.99	>1M - 10M	>1M - 10M	Might be P; t-butyl groups; similar structure to BHT; antioxidant; may oxidize rapidly

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

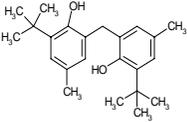
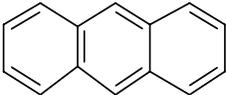
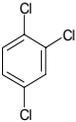
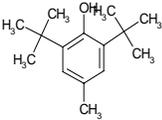
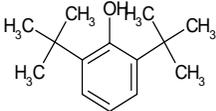
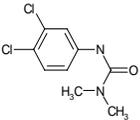
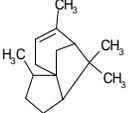
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
000119-47-1		7.97	>1M - 10M	>1M - 10M	Similar to BHT; antioxidant; oxidize rapidly?
000120-12-7		4.35	10K - 500K	No Reports	ESIS profile: P based upon screening studies and soil studies; several studies indicate it biodegrades rapidly; lots of BCF measurements
000120-82-1		3.93	>1M - 10M	>1M - 10M	Maybe be good addition along with 1,2,3-triCl
000128-37-0		5.03	>10M - 50M	>10M - 50M	BHT – antioxidant; oxidizes? Doesn't pass MITI biodegradation test ESIS considers P, but not B
000128-39-2		4.48	>50M - 100M	>100M - 500M	
000128-69-8		6.26	10K - 500K	10K - 500K	Hydrolyzes to tetraacid
000330-54-1		2.67	No Reports	No Reports	
000469-61-4		5.74	No Reports	No Reports	

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

ID	Molstructure	Kowwin	Cus02	Cus06	Comment
000497-39-2		5.88	>1M - 10M	>1M - 10M	Antioxidant
000693-36-7		17.68	>1M - 10M	>1M - 10M	
001103-38-4		6.32	>1M - 10M	>1M - 10M	
001217-08-9		5.62	No Reports	No Reports	ESIS profile: synthetic intermediate for HHCB
001461-25-2		9.37	>10M - 50M	>1M - 10M	
001506-02-1		6.35	No Reports	No Reports	Tonalide: no ESIS profile; might be worth adding; not in earlier musk class
001762-27-2		3.9	No Reports	No Reports	
001843-05-6		6.96	>1M - 10M	>1M - 10M	
002082-79-3		13.41	>10M - 50M	>10M - 50M	

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

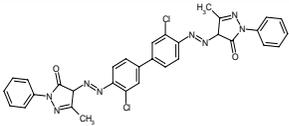
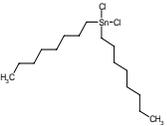
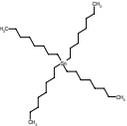
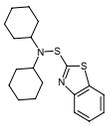
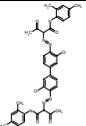
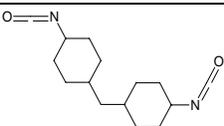
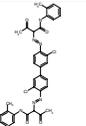
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
003520-72-7		9.55	10K - 500K	10K - 500K	Pigment Orange 13 – disazo pyrazolone (Pyrazolone Orange) coupling tetrazotized 3,3'-dichlorobenzidine with 1-phenyl-3-methylpyrazolone
003542-36-7		5.82	10K - 500K	No Reports	
003590-84-9		17.23	>1M - 10M	No Reports	
004904-61-4		5.48	>50M - 100M	>50M - 100M	
004979-32-2		5.95	>1M - 10M	>1M - 10M	
005102-83-0		8.11	>1M - 10M	>1M - 10M	Pigment Yellow 13 – diarylide - coupling tetrazotized 3,3'-dichlorobenzidine with acetoacet-2,4-dimethyl-anilide
005124-30-1		6.11	>10M - 50M	>10M - 50M	Hydrolyzes very rapidly
005468-75-7		7.02	>1M - 10M	>1M - 10M	Yellow 14

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

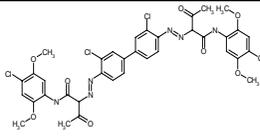
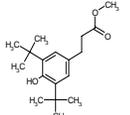
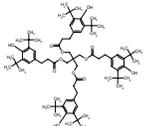
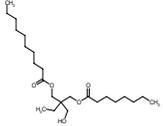
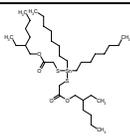
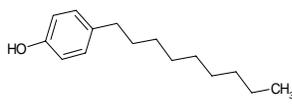
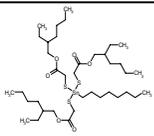
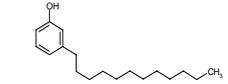
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
005567-15-7		7.54	>1M - 10M	>1M - 10M	Pigment Yellow 83 – diarylide - coupling tetrazotized 3,3'-dichlorobenzidine with acetoacet-2,5-dimethoxy-4-chloroanilide
006386-38-5		5.06	>50M - 100M	>50M - 100M	
006683-19-8		19.6	>10M - 50M	>10M - 50M	
011138-60-6		7.67	>1M - 10M	>1M - 10M	
012578-12-0		14.12	10K - 500K	No Reports	
015571-58-1		15.35	>1M - 10M	>500K - 1M	
025154-52-3	 MIXTURE OF ISOMERS	5.99	No Reports	10K - 500K	
027107-89-7		14.42	>500K - 1M	10K - 500K	
027193-86-8	 MIXTURE OF ISOMERS	7.46	No Reports	No Reports	

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

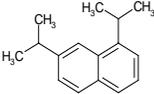
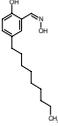
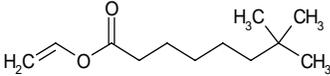
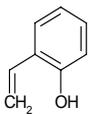
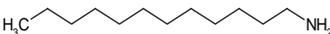
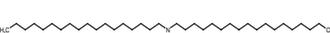
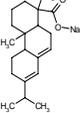
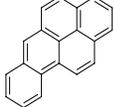
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
038640-62-9	 <p>MIXTURE OF ISOMERS</p>	6.08	10K - 500K	>500K - 1M	
050849-47-3		5.86	>1M - 10M	>1M - 10M	
051000-52-3		4.55	>1M - 10M	>1M - 10M	
061788-44-1		2.41	>500K - 1M	>500K - 1M	
061788-46-3		4.76	>1M - 10M	>10M - 50M	
061789-79-5		16.52	>1M - 10M	>1M - 10M	
061790-51-0		2.65	>10M - 50M	>1M - 10M	
063449-39-8	No Structure		>50M - 100M	>10M - 50M	
064742-04-7		6.11	> 1B	> 1B	

Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

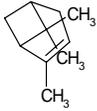
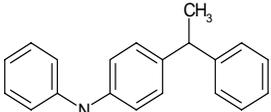
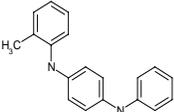
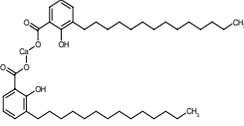
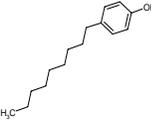
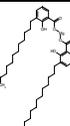
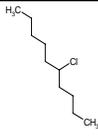
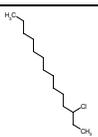
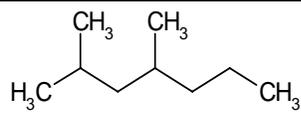
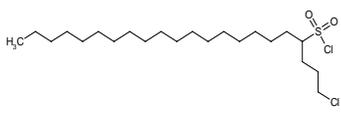
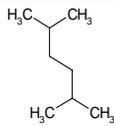
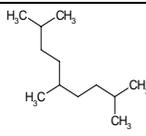
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
065996-93-2	No Structure		>500M - 1B	>500M - 1B	
065996-96-5		4.27	>10M - 50M	No Reports	
068442-68-2		5.45	>1M - 10M	>500K - 1M	
068953-84-4		4.59	>10M - 50M	>10M - 50M	
071786-60-2		3.9			
083846-43-9		16.95			
084852-15-3		5.77	>100M - 500M	>100M - 500M	
084929-98-6		14.98			
084989-41-3		11.25			

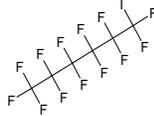
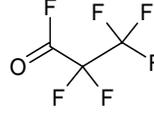
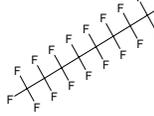
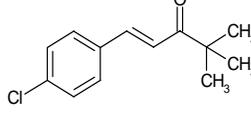
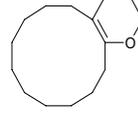
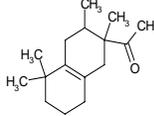
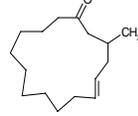
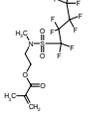
Table 3. Seventy-one PBT Chemicals Listed on the ESIS and DSL/IUR Databases

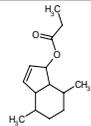
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
085535-84-8		5.43			
085535-85-9		7.4			
090622-57-4		4.61			
090640-80-5	No Structure		10K - 500K	No Reports	
090640-86-1	No Structure		>10M - 50M	No Reports	
091082-32-5		11.77			
093685-78-0		4.12			
093685-81-5		6.01			

With the exception of the lead compounds, the two trichlorobenzene compound and hexabutadiene, all the rest of the chemicals did not fulfill the PBT criteria on the ESIS site or were still under review. Tetraethyl lead (TEL) continues to decrease in production volume but still is reported to be made in 1-10 M lbs per year in 2006. The ESIS summary fact sheet concludes that TEL hydrolyzes to the lead salt which does not meet the PBT criteria. Interestingly, the tetramethyl lead has been rated a PBT but should also hydrolyze like TEL - there is no summary fact sheet. Both 1,2,4-trichlorobenzene (1-10M lbs/yr) and 1,2,3-trichlorobenzene (10-500K lbs/yr) may be good candidates to add to the priority list and have been rated PBTs by ESIS. 1,2,4-Trichlorobenzene has been used as a dye carrier and a substitute for PCBs (K-O) both of which would result in environmental release. Hexachloro-1,3-butadiene (87-68-3) maybe a good chemical to add to the priority list (ESIS has rated it as a PBT), but it is a by-product from chlorinated solvent production and its production volume has decrease considerable. All three of these chlorinated chemicals have been detected in the environment previously. A large number of chemicals in the 71 chemicals list are phenols with tertiary-butyl groups in the 2,6 position. These compounds are generally used as antioxidants (e.g., BHT) and oxidize easily. Therefore, they are not expected to be persistent chemicals. A few chemicals are mercaptobenzothiazoles (95-31-8 and 4979-32-2) and are produced in large quantities for rubber processing (parent compound is degraded in which we may need to consider degradation products). Some compounds are so reactive that they should not be considered for PBT listing (e.g., isocyanides which hydrolyze in seconds [5124-30-1]). Very few of the other compounds seem worth adding either because of lack of production volume or a structure that does not appear very persistent.

IV. SCREENING OF THE CHEMICALS UNIQUE TO THE 2006 IUR

There are 874 chemicals that have first appeared in the 2006 IUR list. Some of the rules for 2006 IUR reporting have changed and effect the amount and type of information available. For example, in previous years only organic chemicals were reported if they were manufactured (including imported) in 10,000 pounds or more. Now manufacturers and importers must report site and manufacturing information for chemicals (including inorganics) that are manufactured (including imported) in amounts of 25,000 pounds or greater at a given site. Additionally, domestic processing and use must be reported for chemicals manufactured in amounts of 300,000 pounds or more at a given site. In 2006, 5,546 organic chemicals were reported of which 2,993 chemicals had reported process/use information and 2,118 chemicals had reported commercial/consumer use information. In addition, 654 inorganic chemicals had reported information. Given the new rules (higher reporting production cutoff), it is understandable that only about 220 new organic chemicals have been reported in 2006. All of the new chemicals were screened to see if there were any potential new emerging contaminants. In Table 4 there is a list of 10 chemicals of interest. There are several perfluorinated compounds and a number of compounds that appear to be fragrances. These will be considered with their chemical class during the use and environmental release analysis. For 2006 IUR chemicals with 300,000 pound production, the processing and use information will be used during the use and environmental release analysis of the five chemical categories.

Table 4. Ten Chemicals of Interest					
ID	Molstructure	Kowwin	Cus02	Cus06	Comment
000355-43-1			No Reports	>1M - 10M	
000422-61-7			No Reports	>500K - 1M	
000507-63-1			No Reports	10K - 500K	
001577-03-3			No Reports	>1M - 10M	
006004-38-2		3.59	No Reports	>500K - 1M	
032539-83-6		6.25	No Reports	>1M - 10M	
054464-59-4		5.18	No Reports	>500K - 1M	Fragrances?
063314-79-4		5.75	No Reports	10K - 500K	New fragrance Musconones 3-methylcyclopentadec-5-en-1-ones
067584-59-2			No Reports	10K - 500K	

ID	Molstructure	Kowwin	Cus02	Cus06	Comment
068912-13-0		3.34	No Reports	>500K - 1M	