Supplementary Material (ESI) for Journal of Environmental Monitoring

In Silico Screening for Unmonitored, Potentially Problematic High Production Volume (HPV) Chemicals Prone to Sequestration in Biosolids

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Supplemental Figures (2)

Supplemental Tables (2)

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(A)

Log K_{ow}	Fraction of mass in sludge (%)			p_{fit} ** ($\times 10^{-6}$)
	Experimental	Model A *	Model B **	
0.91 (1)	0.2	0.0	0.0	6.51
2.45 (4)	0.6	0.2	0.2	6.51
3.13 (1)	11; 4	0.9	0.9	6.46
3.16 (3)	1	0.9	0.9	6.46
3.67 (1)	6	3.0	2.9	6.46
4.01 (1)	10; 1	6.3	6.3	6.54
4.8 (2)	30; 50	29.1	21.4	4.74
4.9 (2)	76	34.1	24.7	4.12
5.7 (5)	80; 67	76.5	78.2	7.14
5.76 (6)	43.5; 57.4; 93.5	78.9	85.6	10.4
5.9 (5)	48; 72	83.8	88.0	9.28
Mean				7.19
Standard error				0.585

* Fraction of mass in sludge was calculated using p_{fit} value of 6.51×10^{-6}, which was estimated using full data set

** Fraction of mass in sludge was calculated using different p_{fit} values, estimated using Jackknife method.

(B)

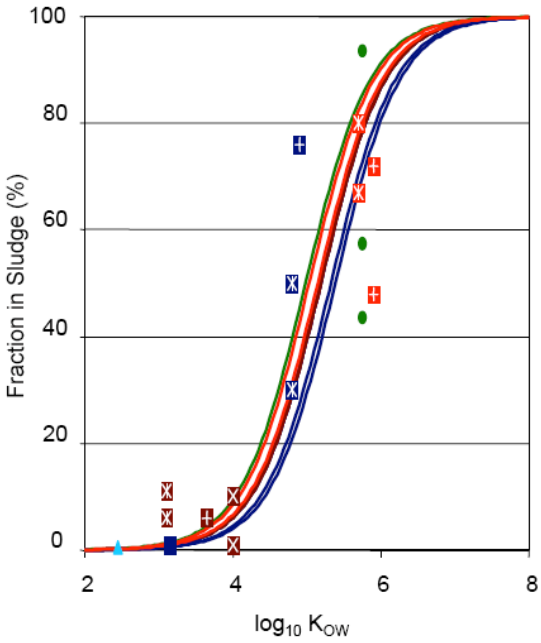

Figure S1. Analysis of cross validation of the empirical model with Jackknife method; (S1A) compares experimental results of fraction of mass in sludge to empirical model A (using full data set fitted single p_{fit} value) and model B (multiple p_{fit} values from reduced data set using Jackknife method); (S1B) compares experimentally determined fraction in sludge to model B. The multiple curves results from using Jackknife estimated individual p_{fit} values to the full dataset. The color of the data points, curves and data in Figure S1A depicts the category of use of the compounds examined, as mentioned in Figure 1.

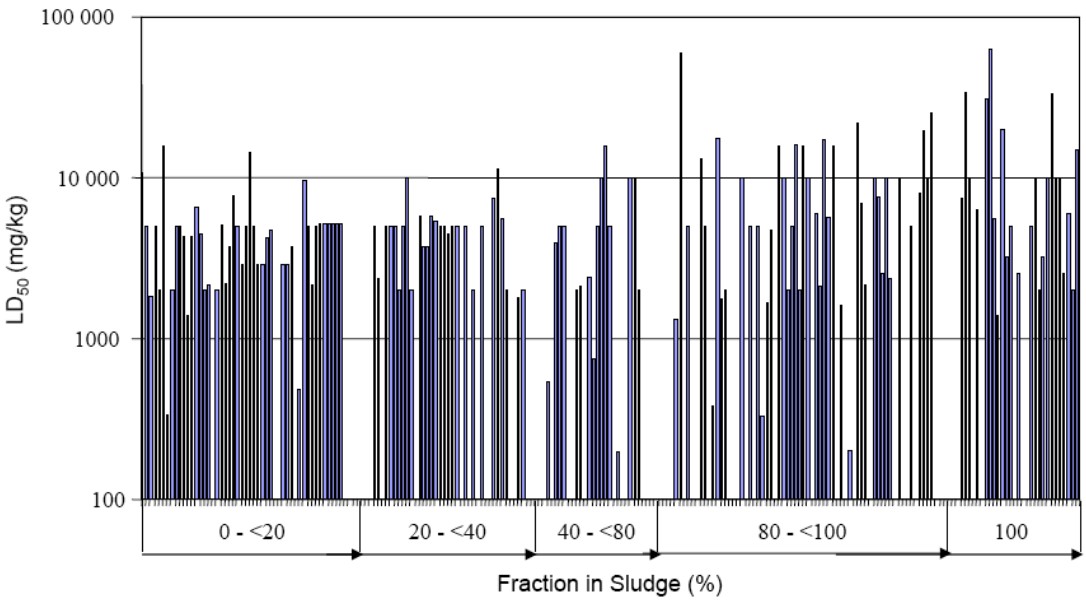

Figure S2. Distribution of the LD_{50} values of HPV chemicals plotted as a function of their mass fraction predicted to accumulate and persist in digested sludge during conventional wastewater treatment.

43 **Table S1.** Chemical Abstract Service (CAS) registry number and logarithmic 1-octanol-
44 water partitioning coefficient (K_{OW}) of organic wastewater compounds for which
45 published mass balances were available for their behavior during wastewater treatment.
46

Compound	CAS #	log K_{OW}
Estrogens		
Estrone	53-16-7	3.13[1]
17β-Estradiol	50-28-2	4.01[1]
17α-Ethinylestradiol	57-63-6	3.67[1]
Antimicrobials		
Triclosan	3380-34-5	4.8[2]
Triclocarban	101-20-2	4.9[2]
Trimethoprim	738-70-5	0.91[1]
Clarithromycin	81103-11-9	3.16[3]
Prescription drugs		
Carbamazepine	298-46-4	2.45[4]
Fragrances		
Galaxolide (HHCB)	1222-05-5	5.9[5]
Tonalide (AHTN)	21145-77-7	5.7[5]
Industrial chemicals		
Nonylphenol	104-40-5	5.76[6]

47 CAS # represents the protonated molecule.

48 **Table S2.** Chemical Abstract Service (CAS) registry number, name, log K_{OW}, LD_{50} and
49 fraction in sludge of HPV chemicals included in this study.
50

CAS#	Name	Use	Log K_{OW}	f_{sludge} (%)	LD_{50} (mg/kg)
68526-53-4	Alkenes, C6-8, C7-rich	I	4.0	6.11	NA
124-19-6	Nonanaldehyde	F/F	4.01	6.25	5000
80-46-6	4-tert-Amylphenol	I	4.03	6.52	1830
125252-49-5	Bicyclo[3.1.1]heptan-2-ol, 2,6,6-trimethyl-, thermal-rearrangement products	F/F	4.09	7.42	2000
68526-82-9	Alkenes, C6-10, hydroformylation products, high-boiling	I	4.11	7.74	15800
599-64-4	4-cumylphenol	I	4.12	7.90	335
118-79-6	2,4,6-Tribromophenol	I	4.13	8.07	2000
108419-33-6	Acetic acid, C8-10-branched alkyl esters, C9-rich	I	4.15	8.42	5000
69013-21-4	Fuel oil, pyrolysis	F/O	4.2	9.35	5000
64741-62-4	Catalytic cracked clarified oils petroleum	F/O	4.2	9.35	4300
80-54-6	Lilial	F/O	4.2	9.35	1390
8002-05-9	Petroleum	F/O	4.2	9.35	4300
2440-22-4	2-(2H-Benzotriazol-2-yl)-p-cresol	I	4.2	9.35	6500
5989-27-5	Citrene	F/F	4.23	9.95	4400
68938-07-8	Fatty acids, C9-13-neo-	I	4.25	10.38	2000
2528-36-1	Dibutyl phenylphosphate	I	4.27	10.81	2140
77-90-7	Acetyl tributyl citrate	I	4.29	11.26	NA
68953-84-4	1,4-Benzenediamine, N,N'-mixed Ph and tolyl derivs.	I	4.3	11.50	2000
80-26-2	Terpinyl acetate (natural)	F/F	4.3	11.50	5075
118-58-1	Benzyl salicylate	F/F	4.31	11.73	2227
122-40-7	Amyl cinnamal	F/F	4.33	12.22	3730
68514-32-9	Hydrocarbons, C10 and C12, olefin-rich	I	4.33	12.22	7740
64742-47-8	Hydrotreated kerosene	F/O	4.35	12.72	5000

68475-80-9	Distillates (petroleum), light steam-cracked naphth	F/O	4.35	12.72	2890
68131-05-5	Hydrocarbon oils, process blends	F/O	4.35	12.72	5000
68513-69-9	Steam cracked light residuum (petroleum)	F/O	4.35	12.72	14500
64742-90-1	Steam cracked residuum pitch (petroleum)	F/O	4.35	12.72	5000
68527-18-4	Steam cracked gas oil (petroleum)	F/O	4.35	12.72	2890
68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. Residues	F/O	4.35	12.72	2890
65996-97-6	Terpenes and Terpenoids, turpentine-oil, .beta.-pinene fraction	F/F	4.35	12.72	4194
127-91-3	Nopinene	F/F	4.35	12.72	4700
473-55-2	Dihydropinene	F/F	4.35	12.72	NA
6876-13-7	cis-Pinane	F/F	4.35	12.72	NA
69430-33-7	Hydrocarbons, C6-30	I	4.35	12.72	2890
68514-34-1	Ethylene by-product distillate, (C9-C14) fraction	F/O	4.35	12.72	2890
68409-73-4	Distilled hydrodealkylized toluene (ECL)	F/O	4.35	12.72	3700
12113-07-4	Sodium hydroxytriphenylborate	I	4.37	13.24	NA
68227-46-3	Propanoic acid, 2-hydroxy-, compd. with 2-ethylhexyl N-[3-[[[2-(dimethylamino)ethoxy]carbonyl] amino]-4-methylphenyl]carbamate (1:1)	I	4.38	13.51	489
26761-45-5	Epoxide 248	I	4.4	14.05	9600
68412-04-4	Acetylated myrcene	F/F	4.48	16.43	5000
84605-28-7	Phosphorodithioic acid, mixed O,O-bis(1,3-dimethylbutyl and iso-Pr) esters	I	4.48	16.43	2140
128-39-2	2,6-Di-tert-butylphenol	I	4.48	16.43	5000

68477-53-2	Distillates (petroleum), steam-cracked, C5-12 fraction	I	4.55	18.76	5175
68603-02-1	Distillates (petroleum), thermal cracked naphtha and gas oil, dimerized	I	4.55	18.76	5175
68527-24-2	Naphtha (petroleum), light steam-cracked arom., C5-12 cycloalkadiene fraction, polymers	I	4.55	18.76	5175
68478-08-0	Naphtha (petroleum), light steam-cracked, C5-fraction, oligomer conc.	I	4.55	18.76	5175
68527-26-4	Naphtha (petroleum), light steam-cracked, debenzenized	I	4.55	18.76	5175
68478-10-4	(C8-C16) Cyclodiene concentrate	I	4.55	18.76	5175
2050-08-0	Amyl salicylate	F/F	4.57	19.48	NA
68526-86-3	Alcohols, C11-14-isoalcs., C13-rich	I	4.6	20.58	NA
131298-44-7	Benzoic acid, C9-11-branched alkyl esters	I	4.61	20.96	5000
68526-55-6	Nonene (petroleum)	I	4.62	21.35	2332
68516-01-8	Phosphorodithioic acid, mixed O,O-bis(iso-Bu and pentyl) esters	I	4.62	21.35	NA
68442-68-2	Styrenated diphenylamine	I	4.64	22.13	5000
68526-54-5	Octene (petroleum)	I	4.65	22.53	5000
108419-34-7	Acetic acid, C9-11-branched alkyl esters, C10-rich	I	4.65	22.53	5000
72480-45-6	Fatty acids, C9-28-neo-	I	4.65	22.53	2000
89331-94-2	ODB-2	I	4.66	22.93	5000
68526-56-7	Decene (petroleum)	I	4.69	24.18	10000
8016-81-7	Tall-oil pitch	F/F	4.7	24.60	2000
65996-96-5	Terpenes and Terpenoids, turpentine-oil, .alpha.-pinene fraction	F/F	4.83	30.56	NA

9005-90-7	Gum turpentine	F/F	4.83	30.56	5760
7785-26-4	Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-, (1S,5S)-	F/F	4.83	30.56	3700
80-56-8	Monoterpenes	F/F	4.83	30.56	3700
8006-64-2	Turpentine oil	F/F	4.83	30.56	5760
138-86-3	Limonene	F/F	4.83	30.56	5300
1335-46-2	Methylionone	F/F	4.84	31.05	5000
220352-35-2	butylated triphenyl phosphate	I	4.85	31.55	5000
586-62-9	Terpinolene	F/F	4.88	33.06	4390
2436-90-0	Citronellene	F/F	4.88	33.06	5000
123-35-3	Myrcene	F/F	4.88	33.06	5000
68955-98-6	Fatty acids, C16-18 and C18-unsatd., branched and linear	F/F	4.9	34.09	NA
64743-00-6	Hydrocarbon waxes (petroleum), oxidized	I	4.9	34.09	5000
68602-85-7	Hydrocarbon waxes (petroleum), oxidized, Me esters	I	4.9	34.09	NA
68603-10-1	Hydrocarbon waxes (petroleum), oxidized, Me esters, barium salts	I	4.9	34.09	2000
68603-11-2	Hydrocarbon waxes (petroleum), oxidized, Me esters, calcium salts	I	4.9	34.09	NA
64743-01-7	Petrolatum (petroleum), oxidized	I	4.9	34.09	5000
68425-34-3	Petrolatum (petroleum), oxidized, calcium salt	I	4.9	34.09	NA
68153-38-8	Resin acids, esters with diethylene glycol	I	4.9	34.09	NA
99-62-7	m-DIISOPROPYLBENZENE	I	4.9	34.09	7400
100-18-5	p-DIISOPROPYLBENZENE	I	4.9	34.09	11540
25321-09-9	DIISOPROPYLBENZENE	I	4.9	34.09	5556.8
71808-39-4	Fatty acids, C16-18 and C18-unsatd., dimerized	I	4.95	36.72	2000
68649-83-2	Resin acids and Rosin acids, fumarated, potassium salts	I	4.95	36.72	NA

68784-30-5	Phosphorodithioic acid, mixed O,O-bis(sec-Bu and 1,3-dimethylbutyl) esters	I	4.97	37.79	NA
4904-61-4	1,5,9-Cyclododecatriene	I	4.97	37.79	1780
72624-02-3	Phenol, heptyl derivs.	I	5.01	39.98	2000
155-04-4	Mercaptobenzothiazole zinc salt	I	5.02	40.54	540
61790-51-0	Resin acids, sodium salts	I	5.05	42.21	NA
65997-06-0	Rosin, hydrogenated	F/F	5.05	42.21	4000
68987-42-8	Polyethylbenzene residue	I	5.05	42.21	5000
1330-61-6	Isodecyl propenoate	I	5.07	43.34	5000
68152-92-1	Tall oil, disproportionated	F/F	5.15	47.90	NA
68783-82-4	Rosin, low-boiling fraction	I	5.15	47.90	NA
68425-08-1	Rosin, distn. Overheads	I	5.15	47.90	2000
3081-01-4	Santoflex 14	I	5.17	49.05	2100
68647-72-3	Sweet orange oil terpenes	F/F	5.3	56.50	NA
96-76-4	2,4-Di-t-butylphenol	I	5.33	58.19	2400
3081-14-9	Eastozone	I	5.34	58.75	750
68411-58-5	2,5-Furandione, 3-(dodecenyl)dihydro-, reaction products with propylene oxide	I	5.36	59.86	5000
68514-33-0	Hydrocarbons, C12 and C14, olefin-rich	I	5.37	60.41	10000
29761-21-5	Isodecyl diphenyl phosphate	I	5.44	64.20	15800
68937-41-7	Isopropylated triphenyl phosphate	I	5.44	64.20	5000
1806-26-4	p-Octylphenol	I	5.5	67.31	NA
960-71-4	Triphenylboron	I	5.52	68.31	196
26472-00-4	Dimethyldicyclopentadiene	I	5.6	72.16	7700
68526-57-8	Undecene (petroleum)	I	5.61	72.62	NA
3194-55-6	Hexabromocyclododecane	I	5.625	73.30	10000
632-79-1	Bromophthal	I	5.63	73.52	10000
65997-04-8	Rosin, fumarated	I	5.7	76.54	2000
68140-16-9	Tall-oil pitch, sodium salt	F/F	5.8	80.42	NA
68201-37-6	Octadecanoic acid, branched and linear	F/F	5.85	82.17	NA
6028-47-3	Bis(1,3-dimethylbutyl) dithiophosphate	I	5.88	83.16	NA
84852-15-3	p-Nonylphenol	I	5.92	84.41	1300
3319-31-1	Staflex TOTM	I	5.94	85.01	60000

64365-17-9	Resin acids, hydrogenated, esters with pentaerythritol	I	5.95	85.30	NA
70024-69-0	Benzenesulfonic acid, mono-C16-24-alkyl derivs., calcium salts	I	6	86.68	5000
68784-32-7	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu) esters	I	6.02	87.21	NA
113706-14-2	Phosphorodithioic acid, mixed O,O-bis(sec-Bu and isooctyl) esters	I	6.02	87.21	NA
26140-60-3	Santowax R	I	6.03	87.46	13200
108419-35-8	Acetic acid, C11-14-branched alkyl esters, C13-rich	I	6.05	87.96	5000
65997-03-7	Rosin light ends	I	6.1	89.13	NA
27090-63-7	1,6-Hexanediamine, N,N,N',N'-tetrabutyl-	I	6.1	89.13	380
61788-32-7	Hydrogenated terphenyls	I	6.13	89.78	17500
143-29-3	Cryoflex	I	6.2	91.16	1746
29512-49-0	N-102	I	6.2	91.16	2000
65997-01-5	Tall oil, sodium salt	F/F	6.25	92.05	NA
68647-71-2	Tall oil, potassium salt	F/F	6.25	92.05	NA
68527-29-7	Tall oil, disproportionated, potassium salt	F/F	6.25	92.05	NA
61790-12-3	Tall oil fatty acids	I	6.25	92.05	10000
61790-44-1	Potassium tallate	I	6.25	92.05	NA
61790-45-2	Sodium tallate	I	6.25	92.05	5000
65997-02-6	Tall oil brine	F/F	6.3	92.85	NA
8002-26-4	Tall oil	F/F	6.3	92.85	5000
120-95-6	2,4-di-tert-pentylphenol	I	6.31	93.00	330
732-26-3	2,4,6-Tri-tert-butylphenol	I	6.39	94.11	1670
17540-75-9	2,6-di-*tert*-4-*sec*-butylPhenol	I	6.43	94.60	4800
68515-50-4	1,2-Benzenedicarboxylic acid, dihexyl ester, branched and linear	I	6.46	94.94	NA

68515-75-3	Hexanedioic acid, di-C7-9-branched and linear alky esters	I	6.48	95.16	15800
36431-22-8	Black XV or 3-(Diethylamino)-6-methyl-7-(2,4-dimethylphenylamino) fluoran	I	6.5	95.37	10000
70321-86-7	2-(2H-benzotriazol-2-yl)-4,6-bis (1 -methyl-l -phenylethyl) phenol	I	6.5	95.37	2000
72275-86-6	Alkenes, C15-18 .alpha.-, reaction products with sulfurized dodecylphenol calcium salt, sulfurized	I	6.6	96.28	5000
10254-57-6	Carbamodithioic acid, N,N-dibutyl-, C,C'-methylene ester	I	6.73	97.22	16000
2772-45-4	2,4-dicumylphenol	I	6.73	97.22	2000
68515-40-2	Alkyl benzyl Phthalate	I	6.74	97.28	15800
71888-89-6	1,2-Benzenedicarboxylic acid, di-C6-8-branched alk	I	6.87	97.97	10000
136-23-2	Butyl zimate	I	7.04	98.62	100
53980-88-4	Cyclocarboxypropyloleic acid	I	7.09	98.77	6000
210555-94-5	p-Dodecylphenol	I	7.17	98.97	2100
68609-97-2	Alkyl (C12, C14) glycidyl ether	I	7.25	99.14	17100
29036-02-0	Quaterphenyl	I	7.28	99.20	5650
68515-44-6	1,2-Benzenedicarboxylic acid	I	7.41	99.41	15800
79-96-9	Phenol, 4,4'-(1-methylethylidene)bis[2-(1,1-dimeth	I	7.46	99.47	40
10595-60-5	Ketimine Ofdiethylenetriamine	I	7.63	99.64	1590
68649-12-7	Hydrogenated trimer and tetramer of decene	I	7.64	99.65	NA
68610-51-5	4-Methylphenol, reaction products with dicyclopentadiene and isobutylene	I	7.67	99.67	200

68649-43-4	Phosphorodithioic acid, O,O-dioctyl ester, branched	I	7.69	99.69	NA
27554-26-3	1,2-Benzenedicarboxylic acid, diisooctyl ester	I	7.73	99.71	22000
32687-78-8	Irganox MD 1024 or 1,2-bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamoyl)hydrazine	I	7.79	99.75	7000
5810-88-8	Phoslex DT 8	I	7.99	99.84	2152.84
26999-29-1	Phosphorodithioic acid, O,O-diisooctyl ester	I	7.99	99.84	NA
112-88-9	1-Octadecene	I	8	99.85	10000
68411-46-1	Benzenamine, N-phenyl-, reaction products with 2,4,4-trimethylpentene	I	8	99.85	7580
184378-08-3	Benzenamine, N-phenyl-, reaction product with isobutylene and 2,4,4-trimethylpentene	I	8	99.85	2500
629-73-2	1-Hexadecene	I	8.06	99.87	10000
96-69-5	4,4'-Thiobis(6-tert-butyl-3-cresol)	I	8.24	99.91	2345
111381-89-6	1,2-Benzenedicarboxylic acid, (C7, C9) branched and linear	I	8.39	99.94	NA
10081-67-1	Benzenamine, 4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]-	I	8.51	99.95	10000
68648-93-1	1,2-Benzenedicarboxylic acid, mixed decyl and hexy	I	8.54	99.96	NA
68515-45-7	1,2-Benzenedicarboxylic acid, dinonyl ester, branched and linear	I	8.6	99.96	NA
115733-08-9	Benzene, C14-C24-branched and linear alkyl derivs,	I	8.9	99.98	5000
76899-35-9	Methyl eicosenoate	I	9	99.98	NA

85-60-9	Phenol, 4,4'-butylidenebis[2-(1,1-dimethylethyl)-5-methyl-	I	9.09	99.99	7940
68425-16-1	Di-tert-nonylpolysulfide	I	9.14	99.99	19638
37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	I	9.14	99.99	10000
13560-89-9	Dechlorane 605	I	9.3	99.99	25000
111381-90-9	1,2-Benzenedicarboxylic acid, heptyl undecyl ester	I	9.37	99.99	NA
32588-76-4	1,2-bis(tetrabromophthalimido)ethane	I	9.797	100.00	7500
68608-77-5	Benzenamine, 2-ethyl-N-(2-ethylphenyl)-, (tripropenyl) derivs.	I	9.84	100.00	34000
311-89-7	Fluosol 43	I	9.98	100.00	10000
111381-91-0	1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear	I	10.28	100.00	NA
41484-35-9	Fenozan 30	I	10.36	100.00	6300
68921-45-9	Benzenamine, N-phenyl-, reaction products with styrene and 2,4,4-trimethylpentene	I	10.38	100.00	NA
68515-43-5	1,2-Benzenedicarboxylic acid, di-C9-C11 branched and linear alkyl esters	I	10.39	100.00	31000
84-77-5	1,2-benzenedicarboxylic acid, didecyl ester	I	10.5	100.00	NA
26741-53-7	Ultranox 626	I	10.9	100.00	5580
101-67-7	4,4'-Dioctyldiphenylamine	I	11.26	100.00	1414
3648-20-2	Di-n-undecyl phthalate	I	11.49	100.00	20000
27251-75-8	1,2,4-benzenetricarboxylic acid, triisooctyl ester	I	11.59	100.00	3200
11138-60-6	Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate	I	11.6	100.00	5000

35074-77-2	Irganox 259	I	11.74	100.00	NA
123-28-4	Antioxidant AS	I	11.79	100.00	2500
85507-79-5	1,2-Benzenedicarboxylic acid, diundecyl ester, branched	I	11.83	100.00	NA
31565-23-8	Pentasulphide, di-tert-dodecyl	I	11.86	100.00	NA
26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	I	11.95	100.00	5000
68515-47-9	1,2-Benzenedicarboxylic acid, di-C11-14-branched a	I	12.25	100.00	10000
10595-72-9	Di(tridecyl) thiodipropionate	I	12.7	100.00	2000
67989-23-5	1,2,4-benzenetricarboxylic acid, decyl octyl ester	I	12.79	100.00	3200
53894-23-8	1,2,4-benzenetricarboxylic acid, triisononyl ester	I	13.06	100.00	10000
7786-17-6	2,2'-methylenebis[4-methyl-6-nonyl-Phenol	I	13.1	100.00	33000
2082-79-3	Antioxidant 1076	I	13.4	100.00	10000
3806-34-6	O,O'-Dioctadecylpentaerythritol bis(phosphite)	I	15	100.00	10000
693-36-7	Antioxidant STDP	I	17.68	100.00	2500
31570-04-4	Irgafos 168	I	18.1	100.00	6000
6683-19-8	Antioxidant 1010	I	23	100.00	2000
29598-76-3	Propanoic acid, 3-(dodecylthio)-, 1,1'-[2,2-bis[[3-(dodecylthio)-1-oxopropoxy]methyl]-1,3-propanediyl] ester	I	24.77	100.00	15000

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