ATMOSPHERIC POLLUTION RESEARCH

SUPPORTING MATERIAL

How many Persistent Organic Pollutants should we expect?

Martin Scheringer [1], Sebastian Strempel [1], Sirja Hukari [1], Carla A. Ng [1], Markus Blepp [2], Konrad Hungerbühler [1]

[1] *Institute for Chemical and Bioengineering, ETH Zürich, 8093 Zürich, Switzerland*
[2] *Öko-Institut, Merzhauser Straße 173, 79100 Freiburg, Germany*

CONTENT

Selection of chemicals S2

Sources of experimental property data S3

Key to Tables S1 to S3 S3

References S4

Table S1. Potential false positives in the "POP group" because of too high BAF values S6

Table S2. Potential POPs: chemicals exceeding the Annex D criteria, of the Stockholm Convention ("POP group") S8

Table S3. Chemicals strongly exceeding the Annex D criteria of the Stockholm Convention ("very-POP group") S72

Corresponding author: *Martin Scheringer*; Tel: *+41 44 632 3062*; E-mail: *scheringer@chem.ethz.ch*

Selection of chemicals

The minimum information about a chemical that is needed for a screening exercise based on estimated property data is the CAS number and the SMILES code [1, 2]. The CAS number specifies the identity of the chemical and the SMILES code describes the chemical structure. We collected CAS numbers and SMILES codes from two large databases: the SMILECAS database, which is included in the EPI Suite software [3], and includes CAS, names and SMILES for 115 346 chemicals [4]; and a database provided by the Joint Research Centre of the European Commission (JRC) that includes CAS and SMILES for 72 561 of the 100 204 chemicals in EINECS, the "European Inventory of Existing Commercial Chemical Substances" [5]. We merged the two sets and obtained a set of approximately 135 000 entries. We then applied the following filters in order to obtain our final set of 93 144 chemical structures:

1. Remove incorrect CAS by check for their compliance with the CAS checksum formula [6]: 7519 cases
2. Remove generic SMILES by creating canonical SMILES [2]: 2457 cases
3. Remove isomers of various groups of POP-like chemicals:
   - 3.1 180 isomers of polychlorinated dibenzodioxins and -furans (PCDD/Fs)
   - 3.2 177 isomers of polychlorinated biphenyls (PCBs)
   - 3.3 15 isomers of polybrominated diphenyl ethers (PBDEs)
   - 3.4 72 isomers of polychlorinated diphenyl ethers (PCDEs)
   - 3.5 31 isomers of polychlorinated naphthalenes (PCNs)
   - 3.6 9 isomers of tetrachloro benzyltoluene (ugilec 141).
4. Remove inorganic and metallorganic chemicals, salts and ionic chemicals: 20 854 cases
5. Remove peroxides (347 cases), epoxides (936 cases), and carboxylic and sulfonic acids (1487 cases) because it is uncertain if Epi Suite results for these chemicals are reliable.
6. Remove chemicals with molecular weight exceeding 1000 g/mol (these are outside the applicability domain of ECOSAR [7]): 343 cases
7. Remove chemicals for which Epi Suite reports that they cannot be processed: 233 cases
8. Remove chemicals for which the biodegradation score from BIOWIN3 is derived from molecular weight alone: 6115 cases.

In total, we removed 40 775 substances in all these steps from our initial collection of chemicals.

Sources of experimental chemical property data

In addition to the estimated property data calculated with EPI Suite, we also gathered experimental property data. Data were retrieved by either downloading them as a file or by setting up a computer program that submitted property queries for all individual CAS numbers. The following data sources were used:

- For **biodegradation** we exploited the Biodeg database [8]. It is important to note here that actual half-life data are needed for the purpose of this study; results from tests for ready biodegradability are not sufficient because they do not show the kinetics of biodegradation in the field.
- For **bioconcentration**, we took data from the BCF database (expbcfkm.db) included in EPI Suite [9]; the BCF training and test datasets included in the T.E.S.T. software of the US EPA [10]; a published list of experimental BCFs [11]; the Aquire ECOTOX database [12]; the experimental BCFs found in the Ecological Categorization Results from the Canadian Domestic Substance List [13]; the CHRIP database [14] of the Japanese National Institute of Technology and Evaluation; and the CEFIC BCF gold standard database [15].
- For **acute and chronic aquatic toxicity,** we exploited the Aquire ECOTOX database, and the experimental toxicity data found in the Ecological Categorization Results from the Canadian Domestic Substance List [13] and in the EnviChem database [16].
- For **octanol-water partitioning** we exploited the K_{ow} database (expkow.db) included in EPI Suite [9].

The data retrieved from these sources were first checked for plausibility and then combined with the estimated property data as descibed in the main text. Details are provided by Strempel et al. [17]

Key to Tables S1, S2, S3

Nr: number; CAS: chemical ID (CAS registry number); SMILES: chemical structure code; Depiction: chemical structure figure.

Half-life biodeg: degradation half-life in water; BCF: bioconcentration factor; BAF: bioaccumulation factor; NOEC/ChV: measured (No Observable Effect Concentration) or estimated (ChV) chronic toxicity; LC50/EC50: Measured or estimated acute toxicity; Half-life air OH: degradation half-life for gas-phase reaction with OH radicals; log K_{ow}: log of the octanol-water partition coefficient, PR: pre-registered in the EU.

References

[1] CAS, 2012. CAS – A division of the American Chemical Society. CAS Registry and CAS Registry Numbers. http://www.cas.org/expertise/cascontent/registry/regsys.html, access March 2012.

[2] Daylight, 2008. SMILES – A Simplified Chemical Language; Daylight Chemical Information Systems, Inc.: 120 Vantis – Suite 550 – Aliso Viejo, CA 92656, 2008, http://www.daylight.com/dayhtml/doc/theory/theory.smiles.html, access March 2012.

[3] US EPA, 2012. Estimation Programs Interface Suite for Microsoft Windows, v 4.10; United States Environmental Protection Agency: Washington, DC, USA, 2011; http://www.epa.gov/opptintr/exposure/pubs/episuite.htm., access March 2012.

[4] Syracuse, 2012. SMILECAS Database, Syracuse Research Corporation; http://www.srcinc.com/what-we-do/product.aspx?id=135, access March 2012.

[5] JRC, 2012. EC Inventory; European Commission Joint Research Centre Institute for Health and Consumer Protection; http://ihcp.jrc.ec.europa.eu/our_labs/computational_toxicology/information-sources/ec_inventory, access March 2012.

[6] CAS (2012) Check Digit Verification of CAS Registry Numbers; CAS – A Division of the American Chemical Society, http://www.cas.org/expertise/cascontent/registry/checkdig.html.

[7] Ecological Structure Activity Relationships (ECOSAR), United States Environmental Protection Agency, 2009. http://www.epa.gov/opptintr/newchems/tools/21ecosar.htm, access March 2012.

[8] SRC BIODEG database; http://srcinc.com/what-we-do/databaseforms.aspx?id=382.

[9] EPI Suite Data; http://esc.syrres.com/interkow/EpiSuiteData.htm.

[10] Quantitative Structure Activity Relationships (QSARs), Risk Management Sustainability Research, USEPA; http://www.epa.gov/nrmrl/std/cppb/qsar/.

[11] Dimitrov, S. Dimitrova, N. Parkerton, T. Combers, M. Bonnell, M. Mekenyan, O. (2005) Baseline model for identifying the bioaccumulation potential of chemicals. SAR QSAR Environ. Res. 16, 531–554.

[12] AQUIRE (AQUatic toxicity Information Retrieval); US EPA; http://cfpub.epa.gov/ecotox/

[13] Ecological Categorization Results from the Canadian Domestic Substance List, Environment Canada; http://webnet.oecd.org/ccrweb/Default.aspx

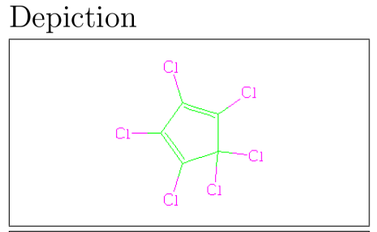
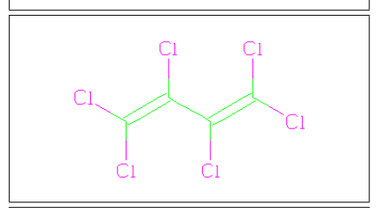
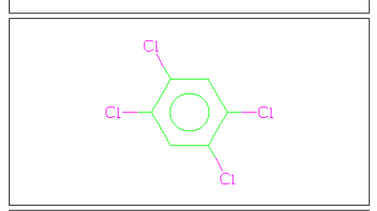
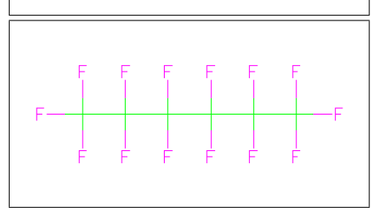
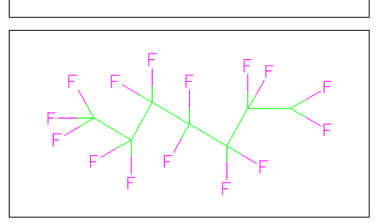
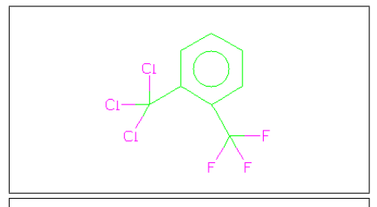
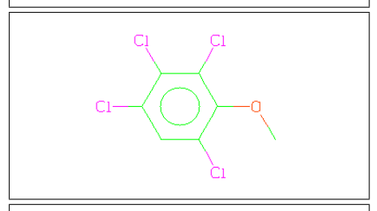
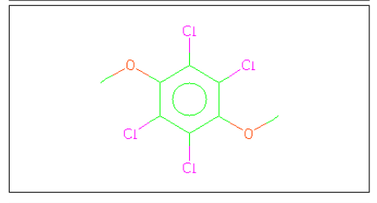
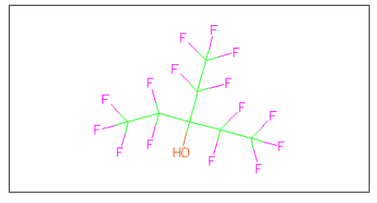
[14] Chemical Risk Information Platform (CHRIP); National Institute of Technology and Evaluation (Japan); http://www.safe.nite.go.jp/english/db.html

[15] BCF gold standard database; CEFIC LRI; http://ambit.sourceforge.net/euras/

[16] Data bank of Environmental Properties of Chemicals – EnviChem; Finish Environment Institute (SYKE); http://www.ymparisto.fi/default.asp?contentid=141944&lan=en

[17] Strempel, S., Scheringer, M., Ng, C.A., Hungerbühler, K. (2012) Screening for PBT chemicals among the “existing” and “new” chemicals of the EU, Environ. Sci. Technol. 46, 5680-5687.

Table S1: Potential false positives in the "POP group" because of too high BAF values

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
1	77-47-4	`ClC1=C(Cl)C(Cl)(Cl)C(=C1Cl)Cl`		$2.23e+02$	$4.31e+01$	$6.50e+03$	$6.00e-03$	$2.03e-02$	$2.72e+01$	4.835	*Yes*
2	87-68-3	`ClC(=C(Cl)C(=C(Cl)Cl)Cl)Cl`		$1.47e+02$	$2.14e+03$	$2.34e+04$	$4.00e-03$	$9.00e-02$	$3.56e+02$	4.75	*Yes*
3	95-94-3	`Clc1cc(Cl)c(Cl)cc1Cl`		$8.56e+01$	$1.97e+03$	$9.64e+03$	$6.00e-03$	$1.45e-01$	$1.30e+02$	4.605	*Yes*
4	355-42-0	`FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.45e+02$	$7.16e+02$	$7.16e+03$	$4.00e-03$	$1.11e-01$	$1.00e+06$	4.83	*Yes*
5	375-83-7	`FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$5.67e+02$	$7.86e+02$	$6.58e+03$	$4.00e-03$	$1.03e-01$	$3.45e+04$	4.89	*No*
6	651-36-5	`FC(F)(F)c1ccccc1C(Cl)(Cl)Cl`		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.98e+02$	4.86	*Yes*
7	938-22-7	`COc1c(Cl)cc(Cl)c(Cl)c1Cl`		$1.06e+02$	$1.18e+03$	$9.59e+03$	$5.00e-03$	$1.32e-01$	$1.07e+01$	4.7	*No*
8	944-78-5	`COc1c(Cl)c(Cl)c(OC)c(Cl)c1Cl`		$1.32e+02$	$6.16e+02$	$2.31e+04$	$5.00e-03$	$1.19e-01$	$4.38e+00$	4.73	*No*
9	6189-00-0	`FC(F)(F)C(F)(F)C(O)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$2.48e+03$	$7.65e+02$	$7.49e+03$	$4.00e-03$	$1.13e-01$	$7.64e+01$	4.88	*No*

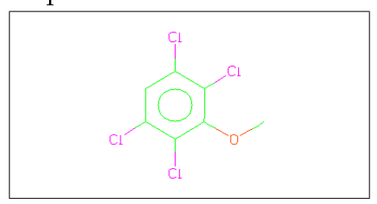
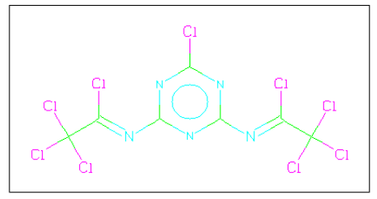
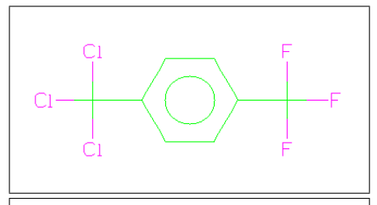
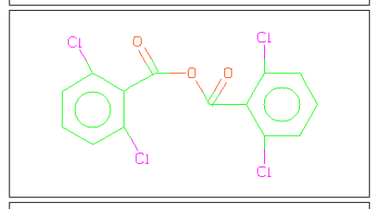
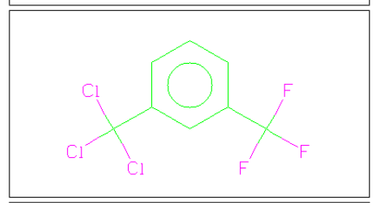
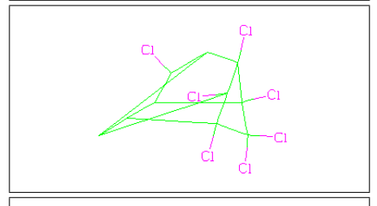
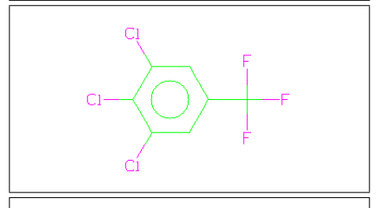
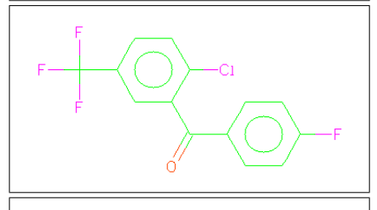
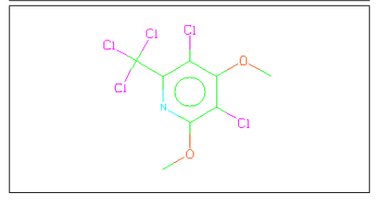
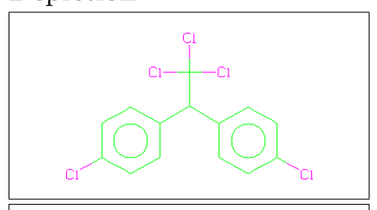
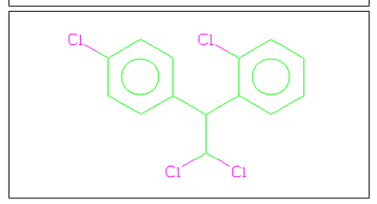
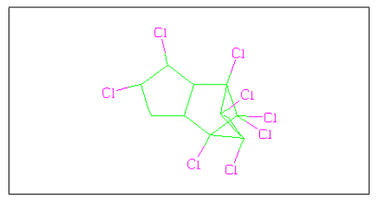
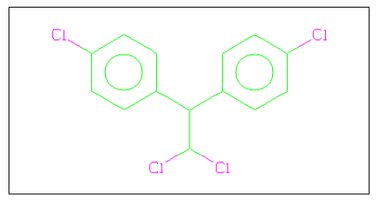
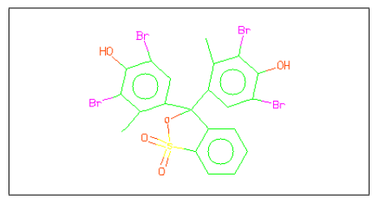
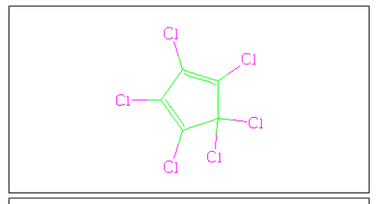
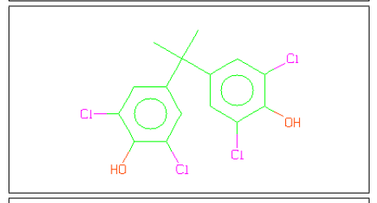
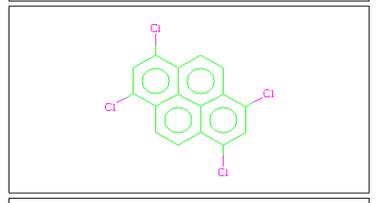
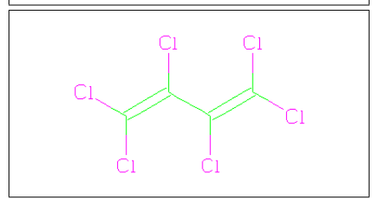
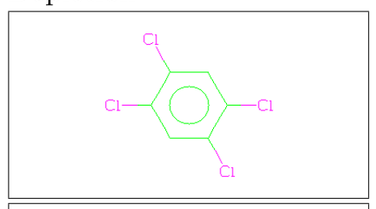
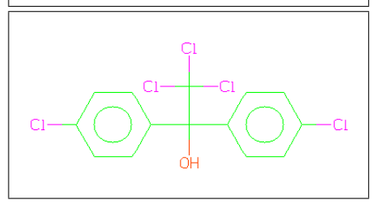
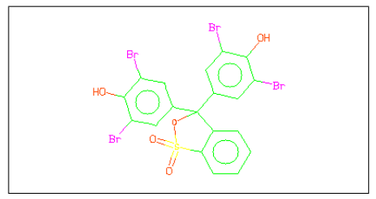
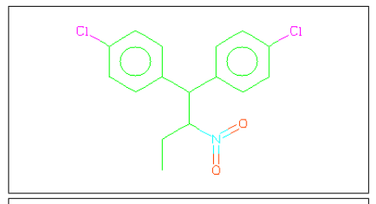
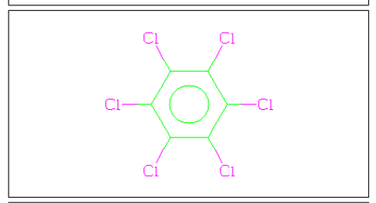
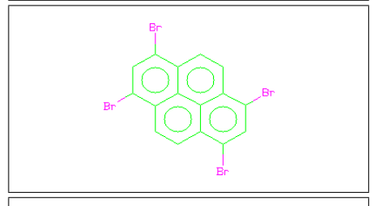
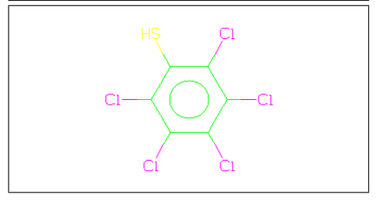
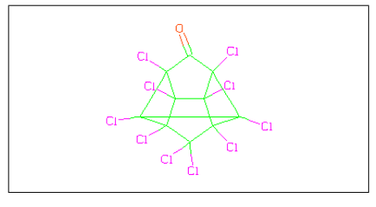
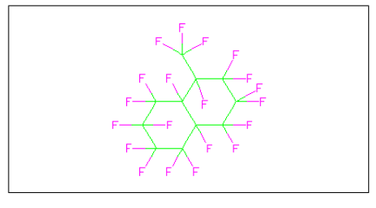
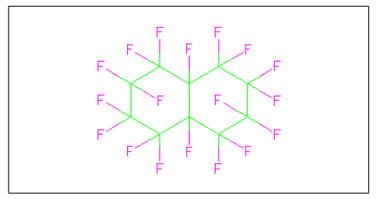
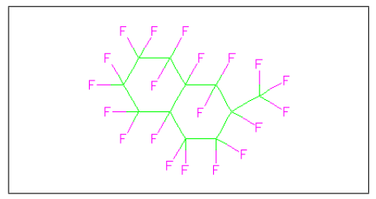
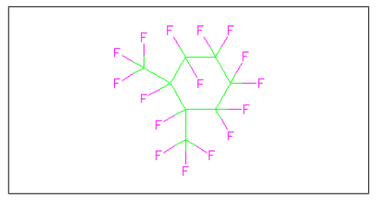
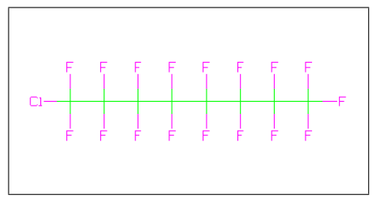
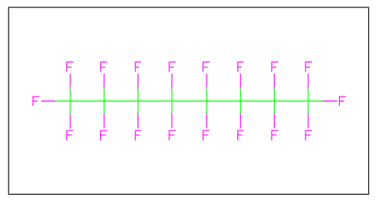
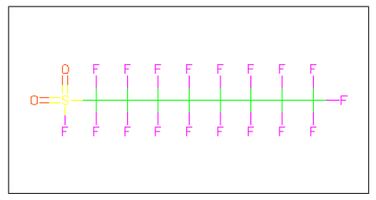
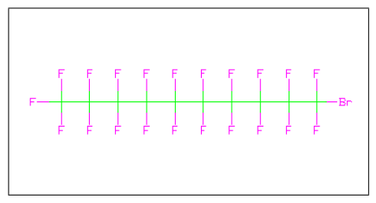
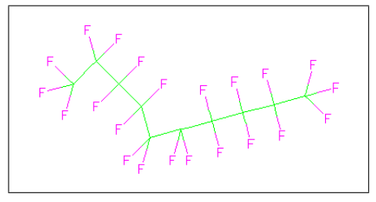
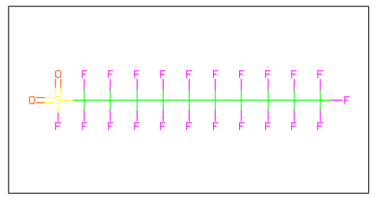
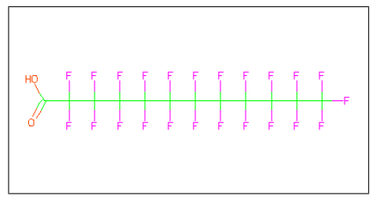
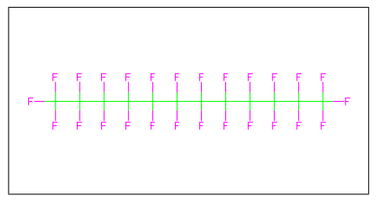
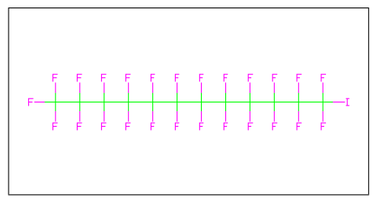
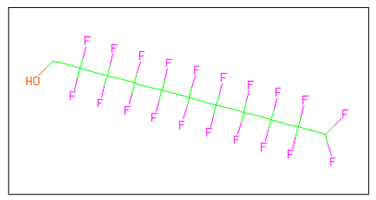
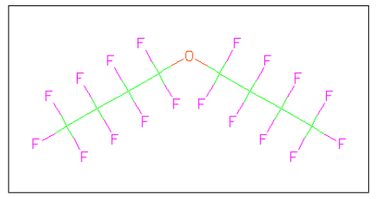
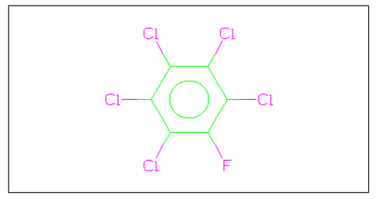
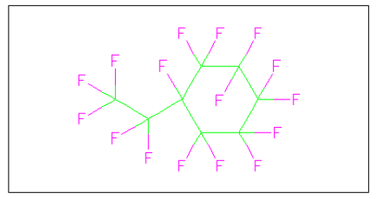
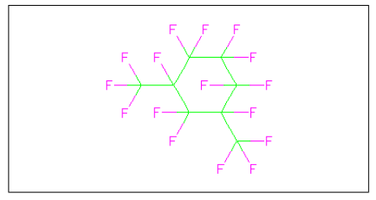
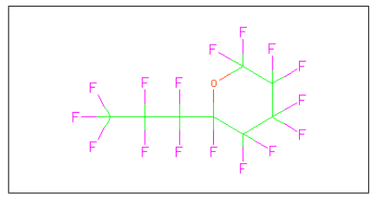
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
10	6936-40-9	`COc1c(Cl)c(Cl)cc(Cl)c1Cl`		$1.06e+02$	$1.67e+03$	$7.55e+03$	$5.00e-03$	$1.32e-01$	$6.16e+00$	4.665	*Yes*
11	10243-83-1	`Clc1nc(nc(n1)N=C(Cl)C(Cl)(Cl)Cl)N=C(Cl)C(Cl)(Cl)Cl`		$2.79e+03$	$2.73e+02$	$1.19e+04$	$9.70e-02$	$4.80e-02$	$2.03e+02$	4.98	*No*
12	13947-96-1	`FC(F)(F)c1ccc(cc1)C(Cl)(Cl)Cl`		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.98e+02$	4.86	*Yes*
13	16442-10-7	`Clc1cccc(Cl)c1C(=O)OC(=O)c1c(Cl)cccc1Cl`		$1.51e+02$	$8.08e+02$	$6.98e+03$	$4.00e-03$	$9.60e-02$	$6.08e+00$	4.91	*Yes*
14	16766-90-8	`FC(F)(F)c1cccc(c1)C(Cl)(Cl)Cl`		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.49e+02$	4.86	*Yes*
15	33442-83-0	`ClC1C2C3C4C1C1(Cl)C2(C1)C(Cl)(Cl)C3(Cl)C41Cl`		$1.93e+03$	$7.73e+02$	$1.43e+04$	$4.00e-03$	$1.07e-01$	$6.77e+00$	4.88	*No*
16	50594-82-6	`Clc1cc(cc(Cl)c1Cl)C(F)(F)F`		$1.66e+02$	$7.82e+02$	$5.36e+03$	$3.00e-03$	$7.00e-02$	$2.51e+02$	4.89	*Yes*
17	85721-08-0	`Fc1ccc(cc1)C(=O)c1cc(ccc1Cl)C(F)(F)F`		$2.09e+02$	$2.24e+02$	$8.48e+03$	$3.00e-03$	$7.10e-02$	$4.32e+00$	4.95	*Yes*
18	108030-77-9	`COc1nc(c(Cl)c(OC)c1Cl)C(Cl)(Cl)Cl`		$4.03e+02$	$5.14e+02$	$6.51e+03$	$5.82e-04$	$1.26e-01$	$4.92e+00$	4.61	*No*

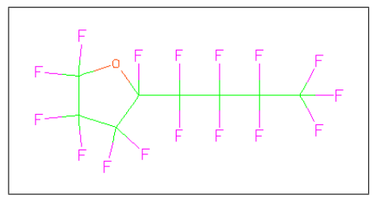
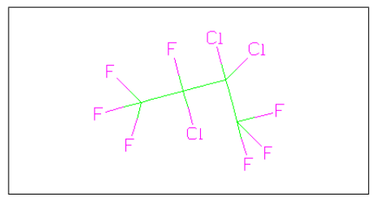
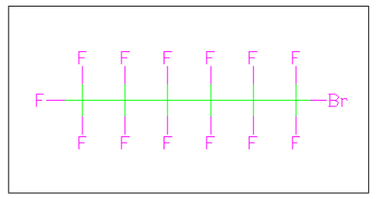
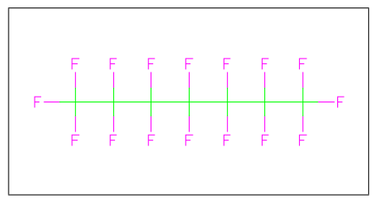
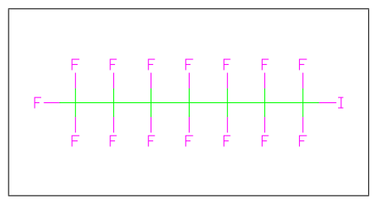
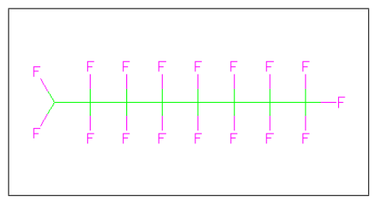
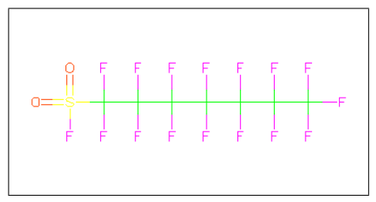
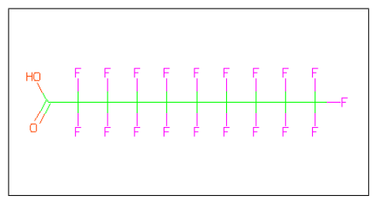
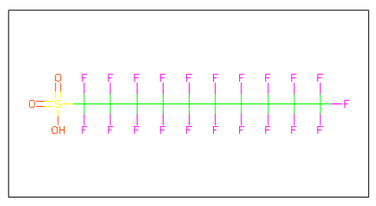
Table S2: Potential POPs: chemicals exceeding the Annex D criteria of the Stockhom Convention ("POP group")

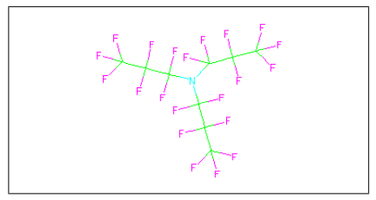
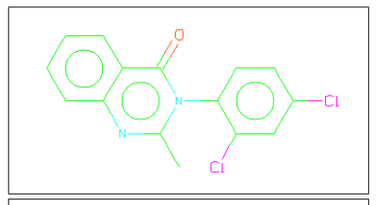
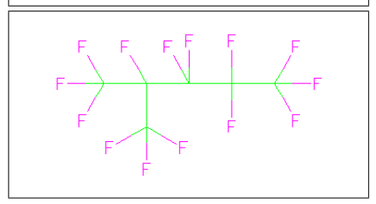
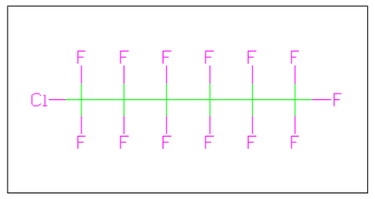
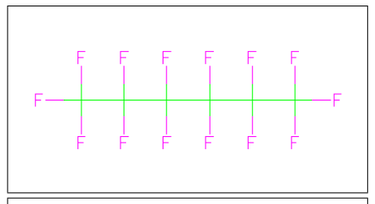
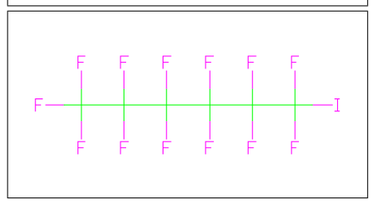
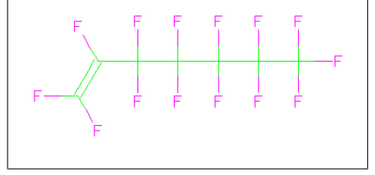
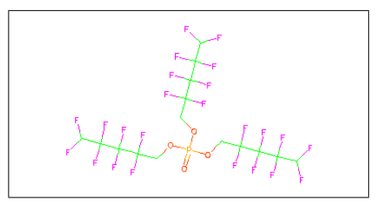
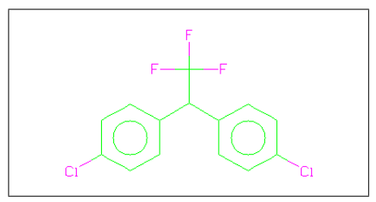
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
1	50-29-3	`Clc1ccc(cc1)C(c1ccc(Cl)cc1)C(Cl)(Cl)Cl`		$2.89e+02$	$2.05e+04$	$2.32e+06$	$1.12e-05$	$2.08e-04$	$3.11e+00$	6.85	*Yes*
2	53-19-0	`Clc1ccc(cc1)C(C(Cl)Cl)c1ccccc1Cl`		$1.30e+02$	$3.49e+03$	$2.07e+05$	$1.66e-04$	$6.00e-03$	$2.46e+00$	5.87	*Yes*
3	57-74-9	`ClC1CC2C(C1Cl)C1(Cl)C(=C(Cl)C2(Cl)C1(Cl)Cl)Cl`		$1.44e+03$	$4.78e+03$	$3.21e+06$	$6.21e-05$	$4.00e-04$	$2.12e+00$	6.24	*Yes*
4	72-54-8	`Clc1ccc(cc1)C(C(Cl)Cl)c1ccc(Cl)cc1`		$1.30e+02$	$3.44e+03$	$1.64e+06$	$1.66e-04$	$6.80e-04$	$2.46e+00$	5.945	*Yes*
5	76-60-8	`Brc1cc(c(C)c(Br)c1O)C1(OS(=O)(=O)c2ccccc12)c1cc(Br)c(O)c(Br)c1C`		$5.14e+02$	$5.04e+03$	$6.85e+02$	$9.79e-07$	$3.00e-03$	$2.46e+00$	7.86	*Yes*
6	77-47-4	`ClC1=C(Cl)C(Cl)(Cl)C(=C1Cl)Cl`		$2.23e+02$	$4.31e+01$	$6.50e+03$	$6.00e-03$	$2.03e-02$	$2.72e+01$	4.835	*Yes*
7	79-95-8	`Clc1cc(cc(Cl)c1O)C(C)(C)c1cc(Cl)c(O)c(Cl)c1`		$1.81e+02$	$5.91e+03$	$1.17e+03$	$7.00e-03$	$7.30e-02$	$3.02e+00$	6.22	*Yes*
8	81-29-8	`Clc1cc(Cl)c2ccc3c(Cl)cc(Cl)c4ccc1c2c34`		$5.53e+02$	$2.88e+04$	$4.00e+03$	$1.23e-06$	$7.26e-05$	$5.07e+00$	7.51	*Yes*
9	87-68-3	`ClC(=C(Cl)C(=C(Cl)Cl)Cl)Cl`		$1.47e+02$	$2.14e+03$	$2.34e+04$	$4.00e-03$	$9.00e-02$	$3.56e+02$	4.75	*Yes*

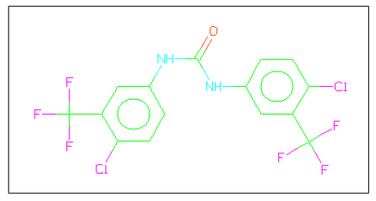
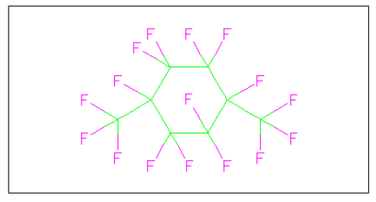
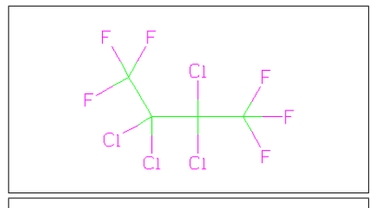
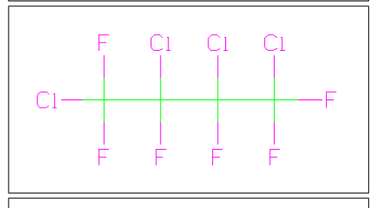
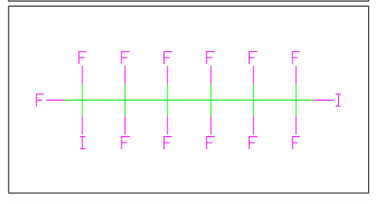
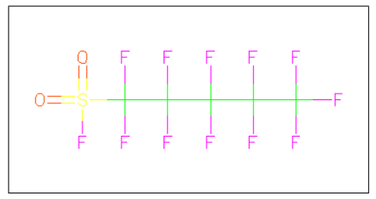
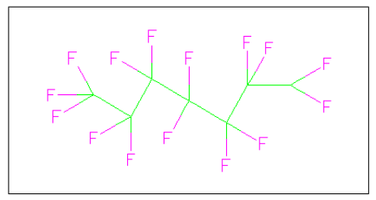
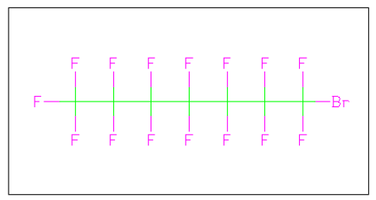
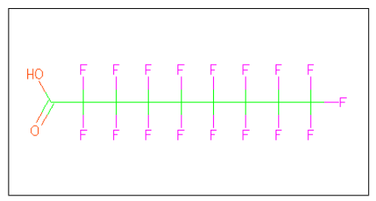
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
10	95-94-3	`Clc1cc(Cl)c(Cl)cc1Cl`		$8.56e+01$	$1.97e+03$	$9.64e+03$	$6.00e-03$	$1.45e-01$	$1.30e+02$	4.605	*Yes*
11	115-32-2	`Clc1ccc(cc1)C(O)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl`		$3.90e+02$	$7.27e+03$	$4.72e+04$	$9.00e-03$	$8.00e-03$	$3.12e+00$	5.415	*Yes*
12	115-39-9	`Brc1cc(cc(Br)c1O)C1(OS(=O)(=O)c2ccccc12)c1cc(Br)c(O)c(Br)c1`		$3.56e+02$	$1.35e+04$	$2.15e+03$	$6.99e-05$	$2.00e-02$	$3.02e+00$	6.77	*Yes*
13	117-26-0	`CCC(N(=O)=O)C(c1ccc(Cl)cc1)c1ccc(Cl)cc1`		$7.21e+01$	$1.91e+03$	$1.18e+04$	$5.59e-04$	$1.80e-02$	$2.67e+00$	5.48	*No*
14	118-74-1	`Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.29e+02$	$1.33e+04$	$7.91e+05$	$1.54e-04$	$2.00e-03$	$1.58e+02$	5.795	*Yes*
15	128-63-2	`Brc1cc(Br)c2ccc3c(Br)cc(Br)c4ccc1c2c34`		$6.70e+02$	$9.52e+03$	$5.55e+02$	$9.47e-08$	$7.50e-06$	$6.57e+00$	8.49	*Yes*
16	133-49-3	`Clc1c(S)c(Cl)c(Cl)c(Cl)c1Cl`		$1.58e+02$	$3.67e+03$	$1.35e+04$	$8.00e-03$	$4.00e-03$	$7.67e+01$	5.91	*Yes*
17	143-50-0	`O=C1C2(Cl)C3(Cl)C4(Cl)C1(Cl)C1(Cl)C2(Cl)C3(Cl)C(Cl)(Cl)C41Cl`		$3.40e+04$	$1.50e+03$	$9.77e+03$	$8.00e-04$	$6.60e-03$	$1.00e+06$	5.16	*Yes*
18	306-92-3	`FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(C1(F)F)C(F)(F)C(F)(F)C(F)(F)C2(F)C(F)(F)F`		$6.17e+03$	$8.63e+03$	$2.37e+06$	$4.35e-05$	$1.89e-03$	$1.00e+06$	6.47	*Yes*

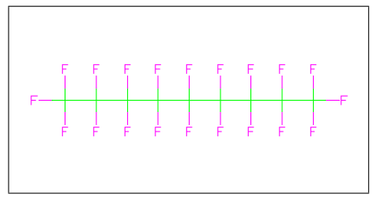
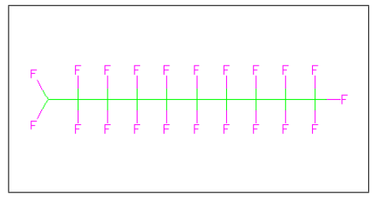
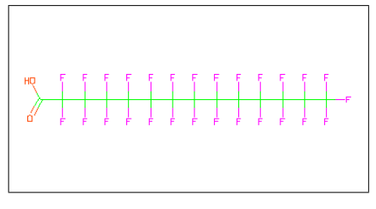
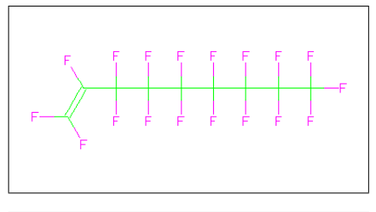
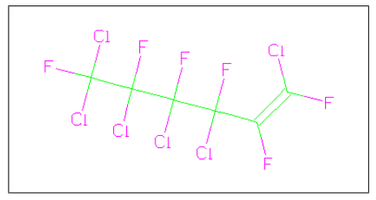
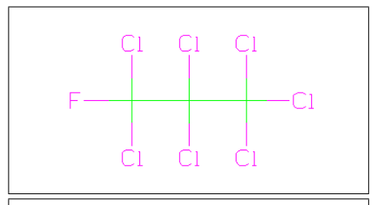
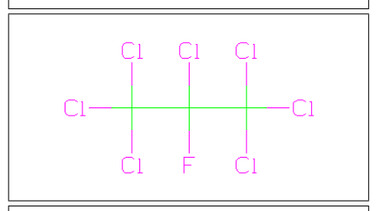
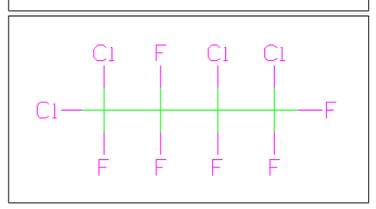
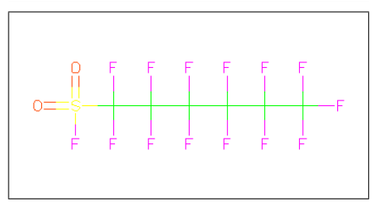
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
19	306-94-5	FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C2(F)C1(F)F		$2.09e+03$	$2.59e+03$	$1.33e+05$	$4.35e-04$	$1.50e-02$	$1.00e+06$	5.68	*Yes*
20	306-95-6	FC1(F)C2(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C1(F)F		$6.17e+03$	$1.33e+04$	$5.44e+06$	$8.67e-06$	$4.41e-04$	$1.00e+06$	7	*Yes*
21	306-98-9	FC1(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(C(F)(F)F)C1(F)F		$2.24e+03$	$1.93e+03$	$3.03e+04$	$6.74e-04$	$2.20e-02$	$1.00e+06$	5.49	*Yes*
22	307-33-5	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Cl)C(F)(F)C(F)(F)F		$2.21e+03$	$8.80e+03$	$2.09e+06$	$3.71e-05$	$1.62e-03$	$1.00e+06$	6.48	*Yes*
23	307-34-6	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.59e+03$	$5.47e+03$	$1.16e+06$	$9.26e-05$	$4.00e-03$	$1.00e+06$	6.17	*Yes*
24	307-35-7	FS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.97e+03$	$5.19e+03$	$4.73e+06$	$3.43e-04$	$4.00e-03$	$1.00e+06$	7.84	*Yes*
25	307-43-7	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br		$5.67e+03$	$4.76e+03$	$6.99e+06$	$6.42e-07$	$4.28e-05$	$1.00e+06$	7.91	*Yes*
26	307-45-9	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$7.96e+03$	$7.50e+03$	$9.73e+06$	$1.96e-06$	$1.16e-04$	$1.00e+06$	7.51	*No*
27	307-51-7	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)F		$6.03e+03$	$1.15e+03$	$1.56e+06$	$5.91e-05$	$3.95e-04$	$1.00e+06$	9.17	*Yes*

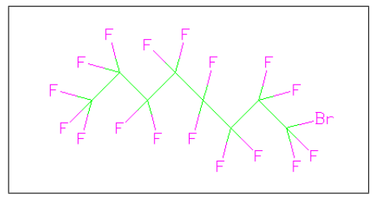
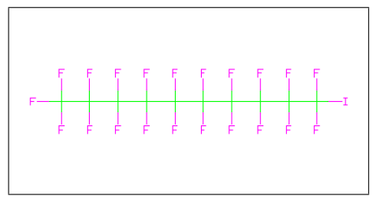
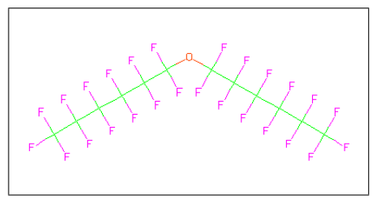
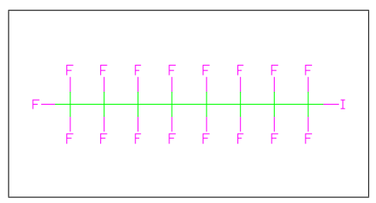
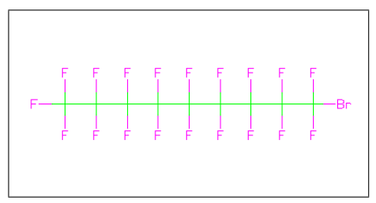
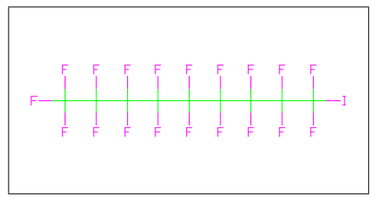
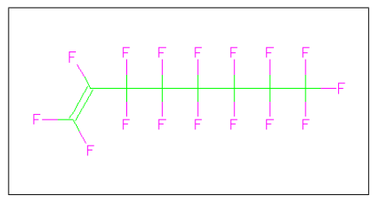
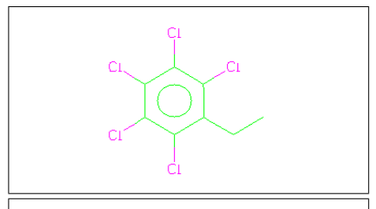
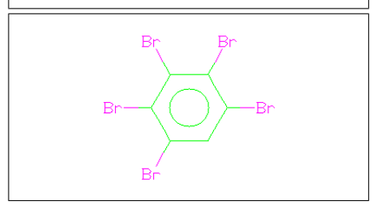
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
28	307-55-1	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$4.85e+03$	$5.62e+01$	$1.01e+07$	$2.35e-05$	$1.39e-03$	$2.06e+01$	7.49	*Yes*
29	307-59-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.44e+04$	$1.66e+03$	$3.86e+06$	$4.00e-08$	$3.51e-06$	$1.00e+06$	8.85	*Yes*
30	307-60-8	FC(F)(I)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.19e+04$	$6.59e+02$	$5.49e+05$	$3.90e-09$	$4.37e-07$	$1.00e+06$	9.66	*Yes*
31	307-70-0	OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.43e+03$	$4.13e+03$	$1.73e+05$	$1.97e-04$	$7.00e-03$	$5.37e+01$	5.99	*Yes*
32	308-48-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.80e+03$	$1.06e+04$	$2.70e+06$	$3.00e-03$	$4.40e-02$	$1.00e+06$	6.61	*No*
33	319-87-9	Clc1c(F)c(Cl)c(Cl)c(Cl)c1Cl		$3.04e+02$	$1.74e+03$	$1.23e+04$	$5.59e-04$	$1.80e-02$	$3.56e+02$	5.42	*No*
34	335-21-7	FC1(F)C(F)(F)C(F)(F)C(F)(C(F)(F)C(F)(F)F)C(F)(F)C1(F)F		$1.33e+03$	$2.52e+03$	$3.43e+04$	$3.98e-04$	$1.40e-02$	$1.00e+06$	5.66	*No*
35	335-27-3	FC1(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C1(F)F		$2.24e+03$	$4.34e+03$	$1.78e+05$	$1.34e-04$	$5.00e-03$	$1.00e+06$	6.02	*Yes*
36	335-35-3	FC(F)(C(F)(F)F)C(F)(F)C1(F)OC(F)(F)C(F)(F)C(F)(F)C1(F)F		$1.43e+03$	$3.58e+03$	$5.57e+04$	$8.00e-03$	$1.51e-01$	$1.00e+06$	5.89	*Yes*

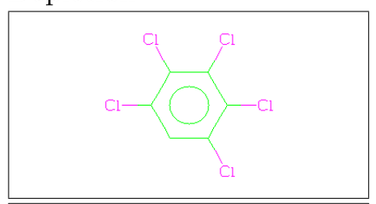
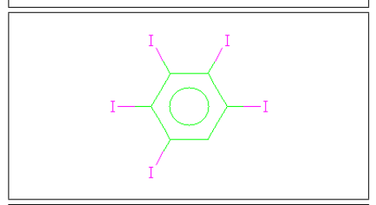
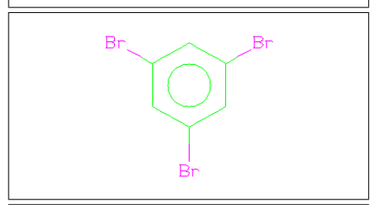
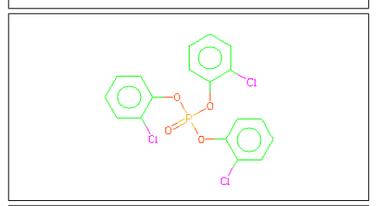
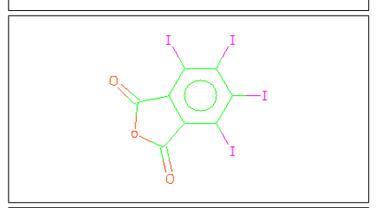
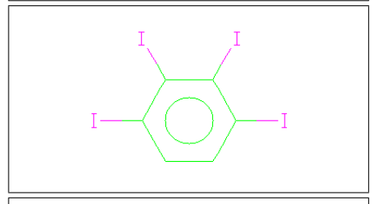
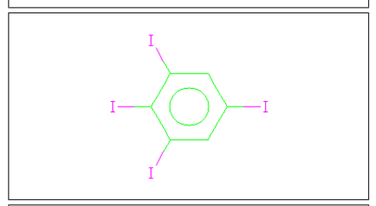
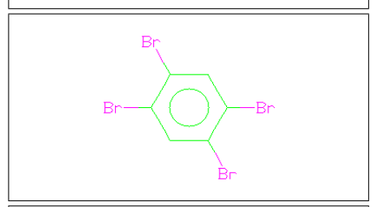
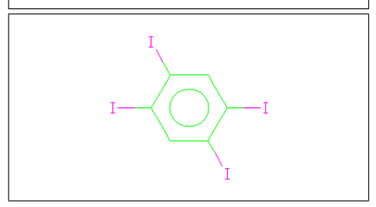
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
37	335-36-4	FC(F)(C(F)(F)C1(F)OC(F)(F)C(F)(F)C1(F)F)C(F)(F)C(F)(F)F		$1.43e+03$	$5.12e+03$	$1.19e+05$	$5.00e-03$	$9.80e-02$	$1.00e+06$	6.13	*Yes*
38	335-44-4	FC(F)(F)C(Cl)(Cl)C(F)(Cl)C(F)(F)F		$8.21e+02$	$9.64e+02$	$9.32e+03$	$1.95e-03$	$5.50e-02$	$1.00e+06$	5.03	*Yes*
39	335-56-8	FC(F)(C(F)(F)Br)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$6.02e+02$	$1.32e+03$	$1.07e+04$	$1.44e-03$	$4.40e-02$	$1.00e+06$	5.23	*Yes*
40	335-57-9	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F		$1.48e+03$	$1.98e+03$	$1.02e+05$	$6.26e-04$	$2.00e-02$	$1.00e+06$	5.5	*Yes*
41	335-58-0	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)F		$1.33e+03$	$6.85e+03$	$1.01e+05$	$6.68e-05$	$3.00e-03$	$1.00e+06$	6.32	*Yes*
42	335-65-9	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$9.93e+02$	$2.17e+03$	$8.92e+04$	$5.62e-04$	$1.90e-02$	$3.45e+04$	5.56	*Yes*
43	335-71-7	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)F		$1.12e+03$	$1.10e+04$	$2.68e+06$	$8.14e-04$	$1.50e-02$	$1.00e+06$	7.17	*Yes*
44	335-76-2	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.58e+03$	$5.62e+01$	$1.24e+06$	$1.15e-03$	$4.50e-02$	$2.06e+01$	6.15	*Yes*
45	335-77-3	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)O		$4.28e+03$	$1.00e+01$	$1.79e+05$	$4.00e-03$	$1.27e-01$	$7.64e+01$	5.83	*Yes*

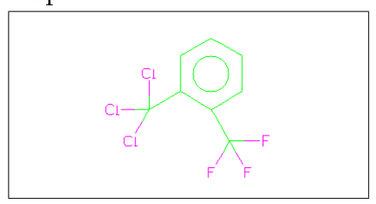
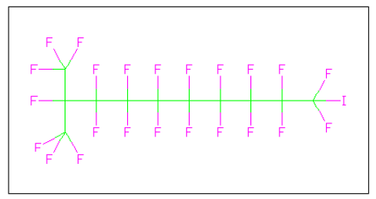
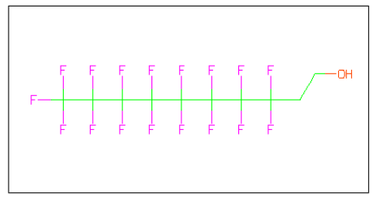
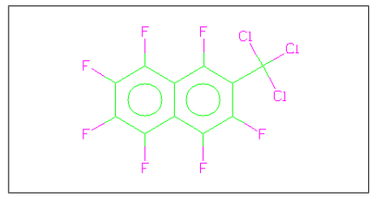
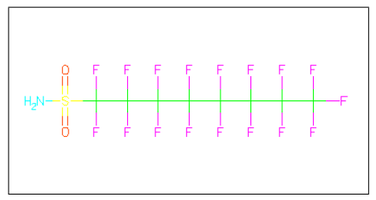
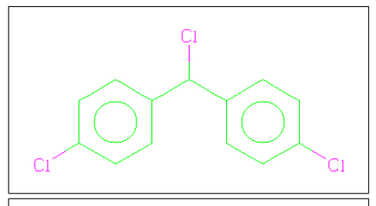
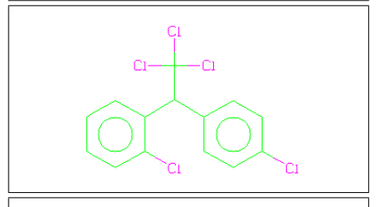
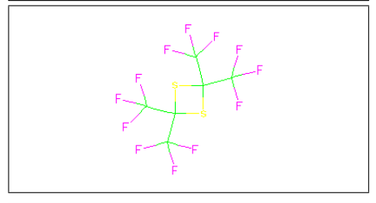
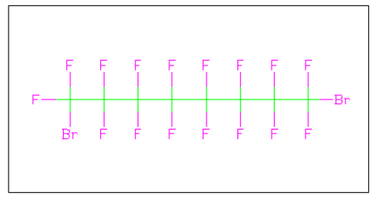
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
46	338-83-0	FC(F)(C(F)(F)F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F		$1.35e+04$	$5.65e+03$	$4.38e+05$	$7.00e-03$	$5.70e-02$	$1.00e+06$	6.19	*Yes*
47	340-53-4	Clc1ccc(c(Cl)c1)n1c(C)nc2ccccc2c1=O		$6.46e+01$	$1.03e+03$	$6.32e+03$	$3.00e-03$	$9.30e-02$	$4.56e+00$	5.07	*No*
48	355-04-4	FC(F)(C(F)(F)F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F		$1.43e+03$	$9.50e+02$	$1.74e+04$	$2.00e-03$	$6.70e-02$	$1.00e+06$	5.02	*Yes*
49	355-41-9	FC(F)(C(F)(F)Cl)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$7.21e+02$	$1.15e+03$	$1.59e+04$	$1.68e-03$	$4.90e-02$	$1.00e+06$	5.14	*Yes*
50	355-42-0	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$8.45e+02$	$7.16e+02$	$7.16e+03$	$4.00e-03$	$1.11e-01$	$1.00e+06$	4.83	*Yes*
51	355-43-1	FC(F)(C(F)(F)I)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$7.59e+02$	$2.48e+03$	$7.30e+03$	$4.58e-04$	$1.60e-02$	$1.00e+06$	5.65	*Yes*
52	355-63-5	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)F		$3.63e+02$	$1.07e+03$	$2.62e+04$	$1.93e-03$	$5.60e-02$	$1.38e+01$	5.1	*Yes*
53	355-86-2	FC(F)C(F)(F)C(F)(F)C(F)(F)COP(=O)(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F		$3.22e+03$	$1.57e+03$	$8.58e+05$	*NA*	$4.56e-03$	$1.03e+01$	7.21	*Yes*
54	361-07-9	Clc1ccc(cc1)C(c1ccc(Cl)cc1)C(F)(F)F		$1.63e+02$	$3.39e+03$	$3.90e+05$	$1.68e-04$	$6.00e-03$	$3.11e+00$	5.85	*No*

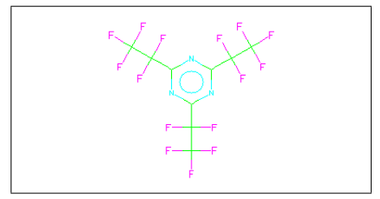
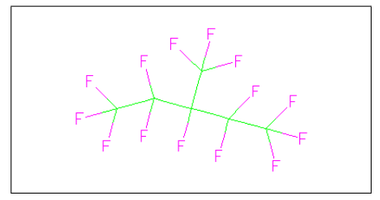
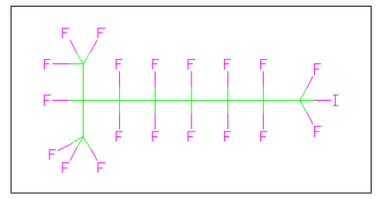
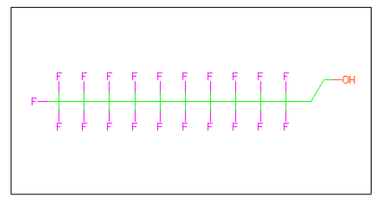
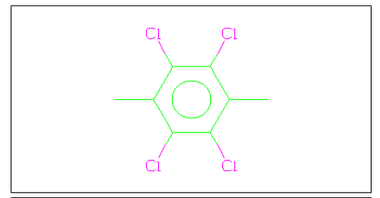
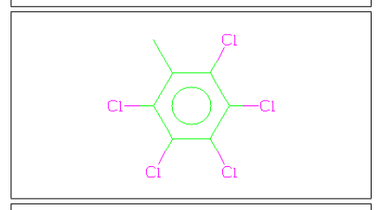
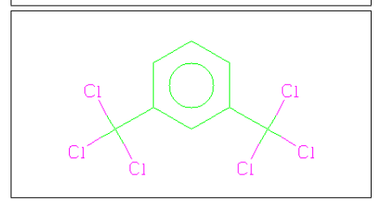
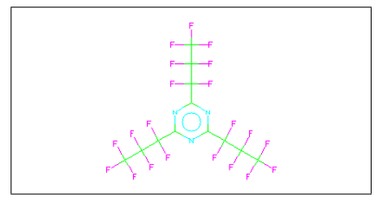
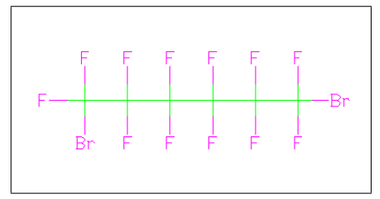
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
55	370-50-3	O=C(Nc1ccc(Cl)c(c1)C(F)(F)F)Nc1ccc(Cl)c(c1)C(F)(F)F		$5.38e+02$	$5.58e+03$	$7.14e+03$	$8.32e-04$	$2.60e-02$	$2.84e+00$	6.18	*Yes*
56	374-77-6	FC1(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C1(F)C(F)(F)F		$2.24e+03$	$9.72e+03$	$7.87e+05$	$2.68e-05$	$1.19e-03$	$1.00e+06$	6.55	*No*
57	375-34-8	FC(F)(F)C(Cl)(Cl)C(Cl)(Cl)C(F)(F)F		$1.18e+03$	$1.55e+03$	$2.95e+04$	$7.96e-04$	$2.50e-02$	$1.00e+06$	5.34	*Yes*
58	375-45-1	FC(F)(Cl)C(F)(Cl)C(F)(Cl)C(F)(F)Cl		$4.16e+02$	$1.55e+03$	$1.31e+04$	$7.96e-04$	$2.50e-02$	$1.00e+06$	5.34	*Yes*
59	375-80-4	FC(F)(I)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$6.81e+02$	$8.59e+03$	$2.37e+03$	*NA*	$1.88e-02$	$1.00e+06$	6.47	*Yes*
60	375-81-5	FS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.66e+02$	$3.25e+03$	$4.10e+04$	$4.00e-03$	$1.43e-01$	$1.00e+06$	5.83	*Yes*
61	375-83-7	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$5.67e+02$	$7.86e+02$	$6.58e+03$	$4.00e-03$	$1.03e-01$	$3.45e+04$	4.89	*No*
62	375-88-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)F		$1.05e+03$	$3.65e+03$	$1.57e+05$	$2.13e-04$	$8.00e-03$	$1.00e+06$	5.9	*Yes*
63	375-95-1	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$9.02e+02$	$1.00e+01$	$1.12e+05$	$8.00e-03$	$2.56e-01$	$2.06e+01$	5.48	*Yes*

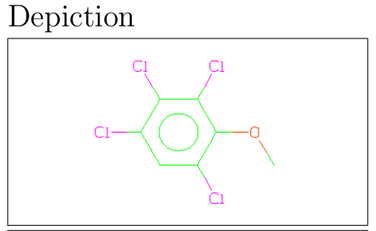
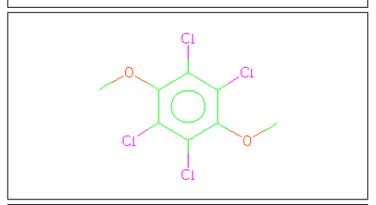
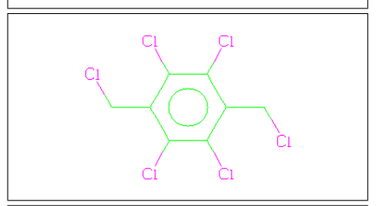
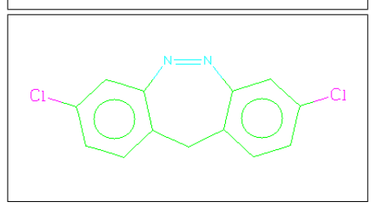
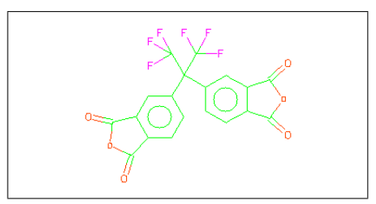
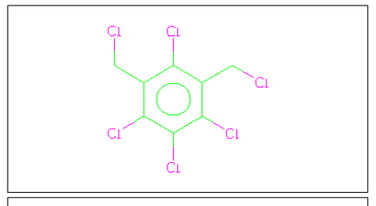
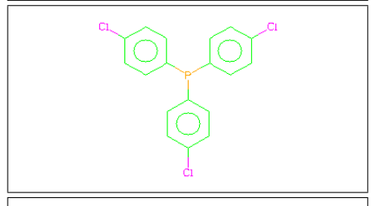
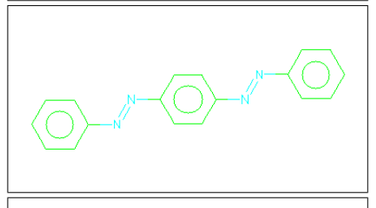
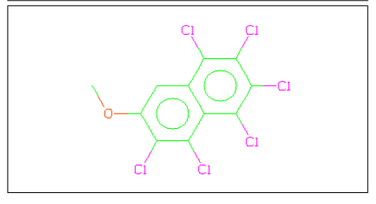
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
64	375-96-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$4.54e+03$	$1.51e+04$	$5.39e+06$	$1.35e-05$	$6.57e-04$	$1.00e+06$	6.84	*No*
65	375-97-3	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.05e+03$	$1.66e+04$	$4.95e+06$	*NA*	$6.55e-03$	$3.45e+04$	6.9	*Yes*
66	376-06-7	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.49e+04$	$1.00e+01$	$4.05e+06$	$4.71e-07$	$4.12e-05$	$2.06e+01$	8.83	*Yes*
67	376-22-7	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)F		$1.11e+03$	$8.17e+03$	$2.89e+06$	*NA*	$1.67e-02$	$1.38e+01$	6.43	*Yes*
68	376-79-4	FC(=C(F)C(F)(Cl)C(F)(Cl)C(F)(Cl)C(F)(Cl)Cl)Cl		$1.09e+03$	$1.29e+04$	$4.90e+06$	$6.06e-06$	$5.80e-04$	$1.38e+01$	7.03	*No*
69	422-78-6	ClC(Cl)(C(F)(Cl)Cl)C(Cl)(Cl)Cl		$7.07e+02$	$1.49e+03$	$1.23e+04$	$8.60e-04$	$2.70e-02$	$1.00e+06$	5.31	*No*
70	422-81-1	ClC(Cl)(Cl)C(F)(Cl)C(Cl)(Cl)Cl		$7.07e+02$	$1.49e+03$	$1.23e+04$	$8.60e-04$	$2.70e-02$	$1.00e+06$	5.31	*No*
71	423-38-1	FC(Cl)(Cl)C(F)(F)C(F)(Cl)C(F)(F)Cl		$4.16e+02$	$1.55e+03$	$1.31e+04$	$7.96e-04$	$2.50e-02$	$1.00e+06$	5.34	*No*
72	423-50-7	FC(F)(C(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)C(F)(F)C(F)(F)F		$6.41e+02$	$8.99e+03$	$5.32e+05$	$1.91e-03$	$4.80e-02$	$1.00e+06$	6.5	*Yes*

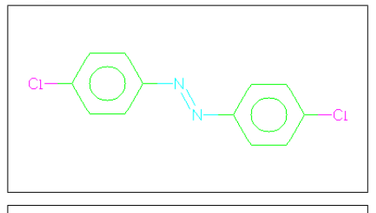
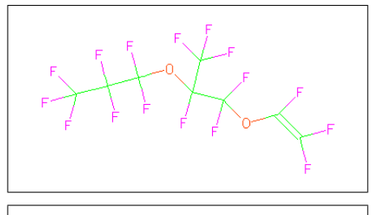
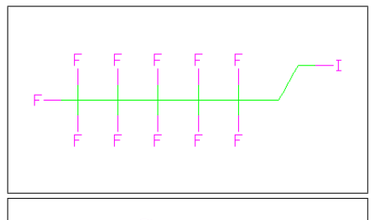
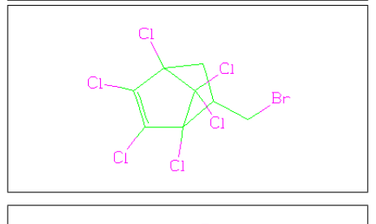
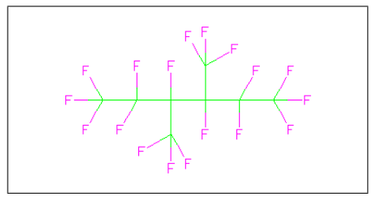
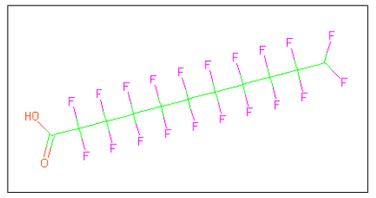
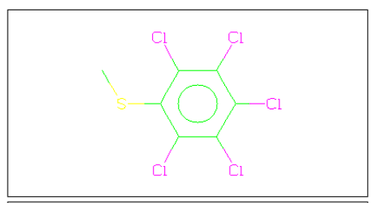
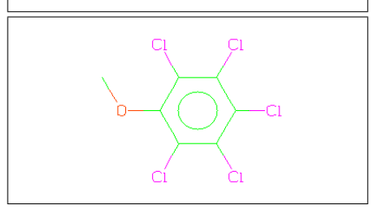
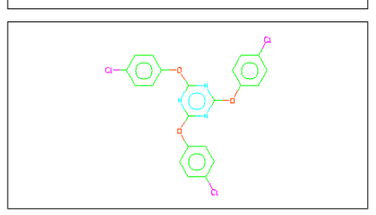
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
73	423-55-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)F		$1.85e+03$	$1.01e+04$	$1.51e+06$	$3.11e-05$	$1.39e-03$	$1.00e+06$	6.57	*Yes*
74	423-62-1	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$7.14e+03$	$2.98e+03$	$2.73e+06$	$1.96e-07$	$1.48e-05$	$1.00e+06$	8.33	*Yes*
75	424-20-4	FC(F)(OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.64e+04$	$1.01e+03$	$1.69e+06$	$4.01e-05$	$3.46e-04$	$1.00e+06$	9.28	*No*
76	507-63-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)F		$2.33e+03$	$1.89e+04$	$8.58e+05$	$9.65e-06$	$4.89e-04$	$1.00e+06$	6.99	*Yes*
77	558-96-3	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)C(F)(F)F		$3.24e+03$	$1.01e+04$	$5.20e+06$	$4.48e-06$	$2.45e-04$	$1.00e+06$	7.24	*No*
78	558-97-4	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)C(F)(F)F		$4.08e+03$	$6.34e+03$	$2.47e+06$	$1.38e-06$	$8.54e-05$	$1.00e+06$	7.66	*Yes*
79	559-14-8	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)F		$6.36e+02$	$2.96e+03$	$3.84e+05$	$2.89e-04$	$1.00e-02$	$1.38e+01$	5.77	*Yes*
80	606-07-5	CCc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl		$1.77e+02$	$6.21e+03$	$6.36e+04$	$4.56e-05$	$1.86e-03$	$9.13e+00$	6.25	*No*
81	608-90-2	Brc1cc(Br)c(Br)c(Br)c1Br		$1.78e+02$	$8.28e+03$	$3.40e+04$	$4.36e-05$	$1.88e-03$	$2.68e+02$	6.44	*No*

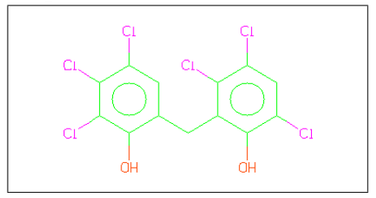
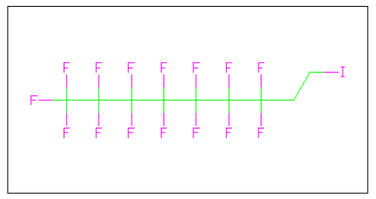
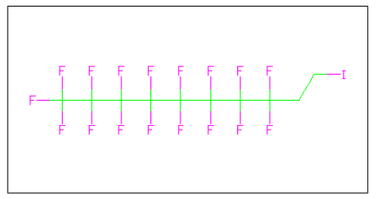
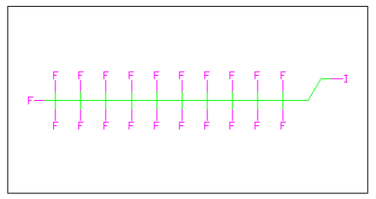
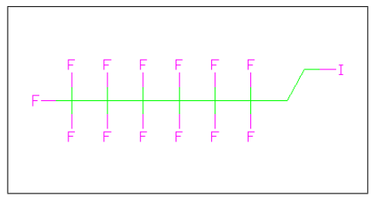
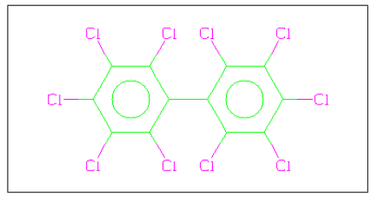
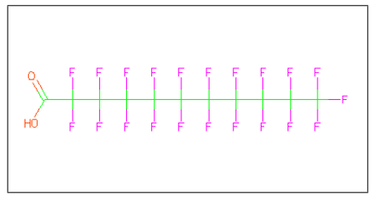
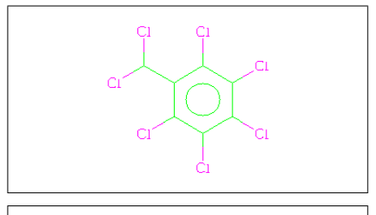
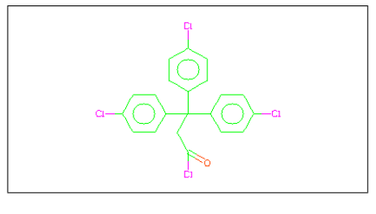
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
82	608-93-5	`Clc1cc(Cl)c(Cl)c(Cl)c1Cl`		$1.37e+02$	$7.09e+03$	$6.19e+04$	$9.59e-04$	$8.94e-03$	$1.85e+02$	5.195	*Yes*
83	608-96-8	`Ic1cc(I)c(I)c(I)c1I`		$1.99e+02$	$5.22e+03$	$5.48e+01$	$9.71e-07$	$6.32e-05$	$1.75e+02$	7.83	*No*
84	626-39-1	`Brc1cc(Br)cc(Br)c1`		$6.05e+01$	$5.62e+03$	$5.25e+03$	$6.00e-03$	$1.64e-01$	$2.20e+01$	4.585	*Yes*
85	631-44-7	`Clc1ccccc1OP(=O)(Oc1ccccc1Cl)Oc1ccccc1Cl`		$1.04e+02$	$1.66e+03$	$1.42e+06$	$3.00e-03$	$1.60e-02$	$3.38e+00$	6.63	*No*
86	632-80-4	`O=C1OC(=O)c2c1c(I)c(I)c(I)c2I`		$1.48e+02$	$1.30e+04$	$1.33e+02$	$2.46e-05$	$1.16e-03$	$3.01e+02$	6.74	*No*
87	634-68-4	`Ic1ccc(I)c(I)c1I`		$1.13e+02$	$1.16e+04$	$2.45e+02$	$2.76e-05$	$1.27e-03$	$1.16e+02$	6.66	*No*
88	634-92-4	`Ic1cc(I)c(I)c(I)c1`		$1.13e+02$	$1.16e+04$	$2.45e+02$	$2.76e-05$	$1.27e-03$	$5.79e+01$	6.66	*No*
89	636-28-2	`Brc1cc(Br)c(Br)cc1Br`		$1.04e+02$	$4.14e+03$	$1.29e+04$	$5.41e-04$	$1.80e-02$	$1.69e+02$	5.34	*Yes*
90	636-31-7	`Ic1cc(I)c(I)cc1I`		$1.13e+02$	$1.16e+04$	$2.45e+02$	$2.76e-05$	$1.27e-03$	$1.16e+02$	6.66	*No*

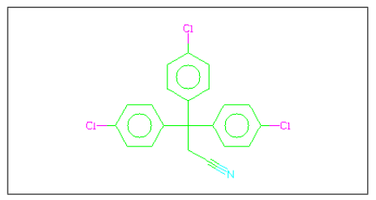
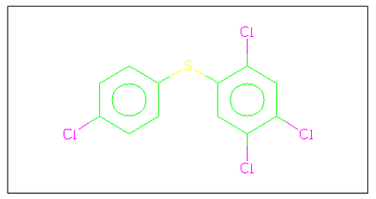
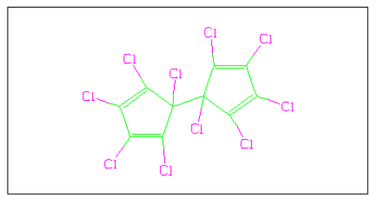
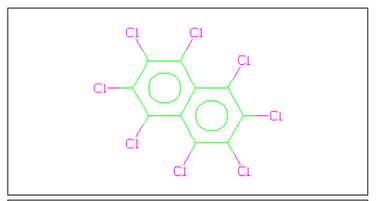
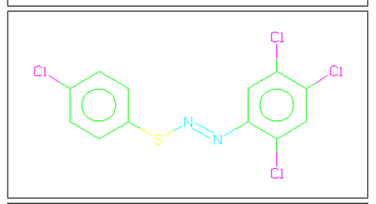
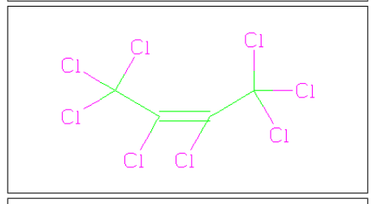
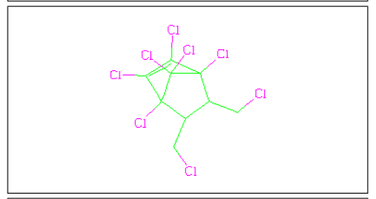
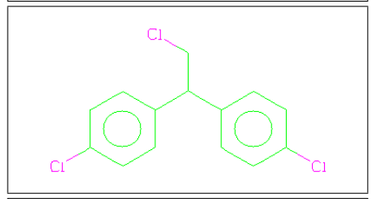
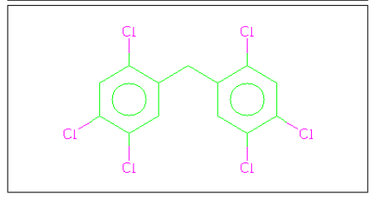
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
91	651-36-5	FC(F)(F)c1ccccc1C(Cl)(Cl)Cl		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.98e+02$	4.86	*Yes*
92	677-93-0	FC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$2.11e+04$	$1.14e+03$	$1.30e+06$	$1.58e-08$	$1.53e-06$	$1.00e+06$	9.18	*Yes*
93	678-39-7	OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.29e+03$	$2.23e+03$	$3.97e+04$	$3.55e-04$	$1.20e-02$	$2.56e+00$	5.665	*Yes*
94	737-20-2	Fc1c(F)c(F)c2c(c1F)c(F)c(F)c(c2F)C(Cl)(Cl)Cl		$1.86e+04$	$8.69e+03$	$3.16e+05$	$9.67e-06$	$4.60e-02$	$6.42e+01$	6.47	*No*
95	754-91-6	NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.94e+03$	$3.13e+03$	$6.06e+04$	$1.75e-03$	$6.30e-02$	$1.00e+06$	5.8	*Yes*
96	782-08-1	Clc1ccc(cc1)C(Cl)c1ccc(Cl)cc1		$6.99e+01$	$1.26e+03$	$1.26e+04$	$1.28e-04$	$7.50e-02$	$4.25e+00$	5.2	*Yes*
97	789-02-6	Clc1ccc(cc1)C(c1ccccc1Cl)C(Cl)(Cl)Cl		$2.89e+02$	$1.41e+04$	$1.07e+06$	$1.12e-05$	$5.39e-04$	$3.11e+00$	6.79	*Yes*
98	791-50-4	FC(F)(F)C1(SC(S1)(C(F)(F)F)C(F)(F)F)C(F)(F)F		$2.66e+03$	$1.43e+04$	$6.48e+05$	$1.13e-05$	$5.41e-04$	$3.15e+00$	6.8	*No*
99	812-58-8	FC(F)(C(F)(F)Br)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br		$1.32e+03$	$1.86e+04$	$1.35e+06$	$1.03e-05$	$5.19e-04$	$1.00e+06$	6.98	*No*

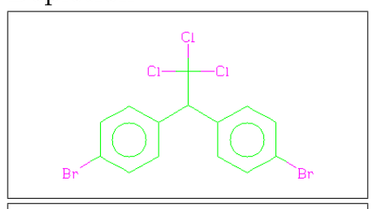
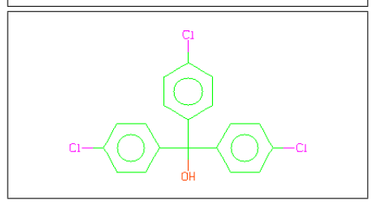
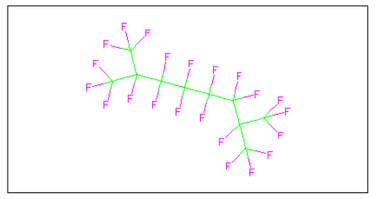
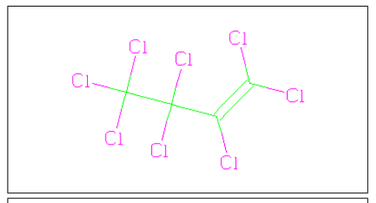
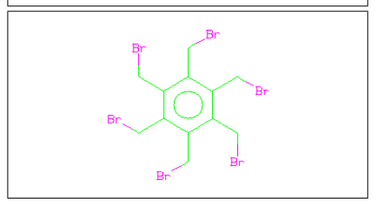
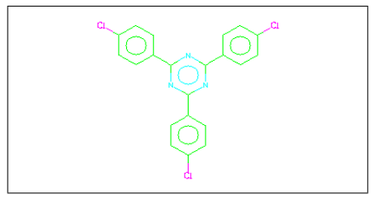
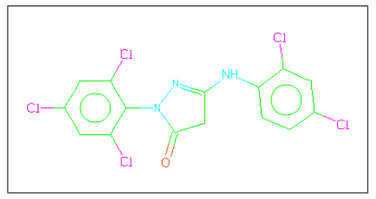
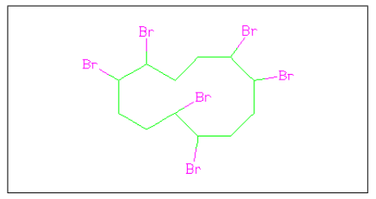
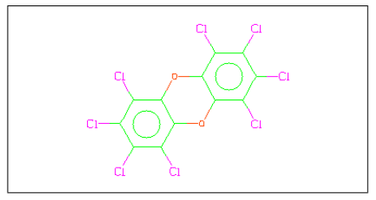
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
100	858-46-8	`FC(F)(F)C(F)(F)c1nc(nc(n1)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$3.17e+03$	$6.86e+02$	$1.38e+05$	$2.70e-02$	$8.00e-03$	$4.13e+01$	5.59	*Yes*
101	865-71-4	`FC(F)(F)C(F)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$1.43e+03$	$1.49e+03$	$5.02e+04$	$9.58e-04$	$3.00e-02$	$1.00e+06$	5.31	*Yes*
102	865-77-0	`FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I`		$6.87e+03$	$5.14e+03$	$3.36e+06$	$7.85e-07$	$5.13e-05$	$1.00e+06$	7.84	*Yes*
103	865-86-1	`OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$3.95e+03$	$1.21e+04$	$3.90e+06$	$7.42e-06$	$3.87e-04$	$2.56e+00$	7.08	*Yes*
104	877-10-1	`Cc1c(Cl)c(Cl)c(C)c(Cl)c1Cl`		$1.24e+02$	$2.51e+03$	$1.49e+04$	$2.38e-04$	$8.00e-03$	$2.00e+01$	5.67	*Yes*
105	877-11-2	`Clc1c(C)c(Cl)c(Cl)c(Cl)c1Cl`		$1.68e+02$	$5.55e+03$	$4.57e+04$	$1.92e-04$	$7.00e-03$	$5.17e+01$	5.69	*No*
106	881-99-2	`ClC(Cl)(Cl)c1cccc(c1)C(Cl)(Cl)Cl`		$3.76e+02$	$3.11e+03$	$1.74e+05$	$3.78e-05$	$6.10e-02$	$1.63e+02$	5.8	*Yes*
107	915-76-4	`FC(F)(C(F)(F)F)C(F)(F)c1nc(nc(n1)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F`		$1.70e+04$	$2.07e+03$	$9.79e+06$	$6.98e-04$	$3.92e-05$	$4.13e+01$	7.59	*Yes*
108	918-22-9	`FC(F)(Br)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br`		$4.29e+02$	$2.43e+03$	$1.21e+04$	$4.90e-04$	$1.70e-02$	$1.00e+06$	5.64	*No*

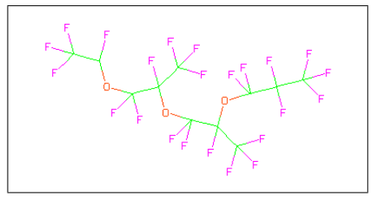
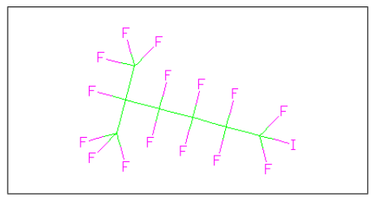
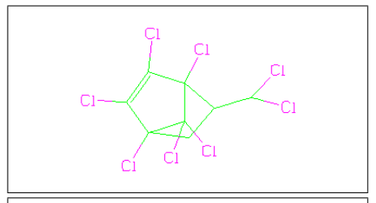
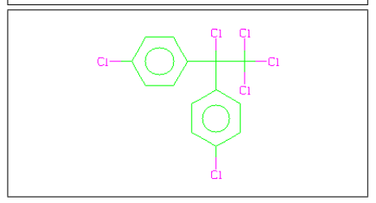
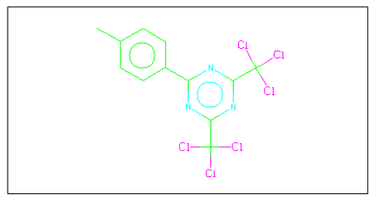
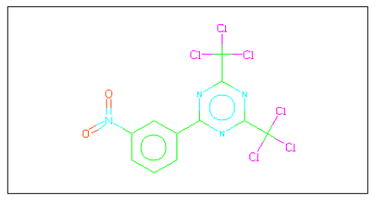
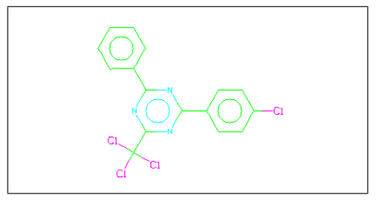
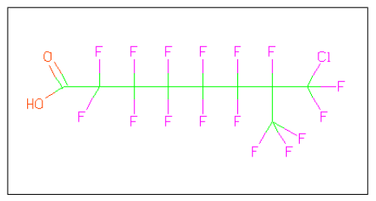
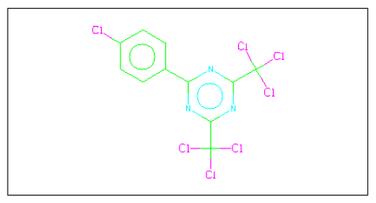
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
109	938-22-7	`COc1c(Cl)cc(Cl)c(Cl)c1Cl`		$1.06e+02$	$1.18e+03$	$9.59e+03$	$5.00e-03$	$1.32e-01$	$1.07e+01$	4.7	*No*
110	944-78-5	`COc1c(Cl)c(Cl)c(OC)c(Cl)c1Cl`		$1.32e+02$	$6.16e+02$	$2.31e+04$	$5.00e-03$	$1.19e-01$	$4.38e+00$	4.73	*No*
111	1079-17-0	`ClCc1c(Cl)c(Cl)c(CCl)c(Cl)c1Cl`		$2.27e+02$	$5.50e+03$	$3.82e+03$	$1.61e-05$	$4.90e-02$	$1.40e+01$	6.17	*Yes*
112	1084-98-6	`Clc1ccc2Cc3ccc(Cl)cc3N=Nc2c1`		$9.61e+01$	$2.52e+03$	$2.23e+04$	$2.62e-04$	$9.00e-03$	$5.20e+00$	5.66	*No*
113	1107-00-2	`O=C1OC(=O)c2cc(ccc12)C(c1ccc2C(=O)OC(=O)c2c1)(C(F)(F)F)C(F)(F)F`		$4.21e+02$	$2.25e+03$	$1.50e+05$	$5.52e-04$	$1.80e-02$	$3.24e+00$	5.59	*Yes*
114	1133-57-9	`ClCc1c(Cl)c(CCl)c(Cl)c(Cl)c1Cl`		$2.27e+02$	$5.50e+03$	$3.82e+03$	$1.61e-05$	$4.90e-02$	$1.35e+01$	6.17	*Yes*
115	1159-54-2	`Clc1ccc(cc1)P(c1ccc(Cl)cc1)c1ccc(Cl)cc1`		$1.06e+02$	$1.80e+04$	$8.40e+06$	$7.14e-06$	$3.58e-04$	$2.60e+00$	6.95	*Yes*
116	1161-45-1	`c1ccc(cc1)N=Nc1ccc(cc1)N=Nc1ccccc1`		$7.02e+01$	$1.00e+01$	$1.06e+04$	$1.34e-05$	$5.37e-05$	$6.47e+00$	6.23	*No*
117	1506-15-6	`COc1cc2c(Cl)c(Cl)c(Cl)c(Cl)c2c(Cl)c1Cl`		$3.44e+02$	$1.17e+04$	$7.46e+06$	$4.35e-06$	$2.29e-04$	$7.60e+00$	7.12	*Yes*

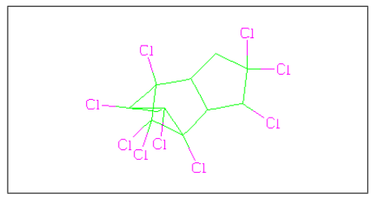
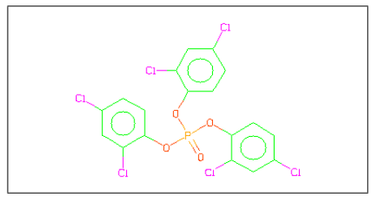
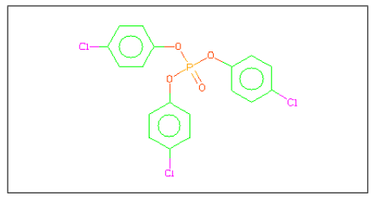
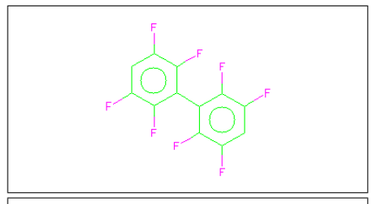
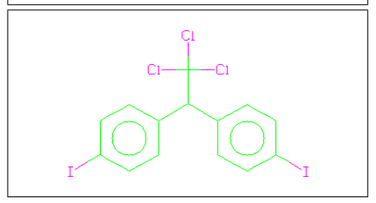
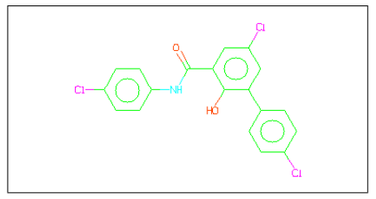
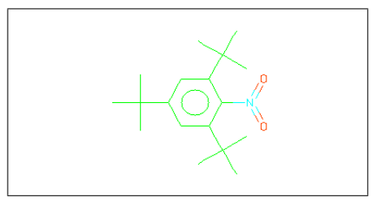
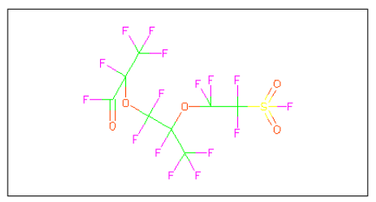
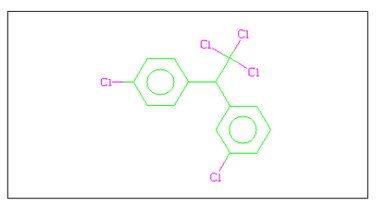
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
118	1602-00-2	`Clc1ccc(cc1)N=Nc1ccc(Cl)cc1`		$8.06e+01$	$1.00e+01$	$4.19e+04$	$1.18e-05$	$4.71e-05$	$9.84e+00$	5.4	*No*
119	1644-11-7	`FC(=C(F)F)OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F`		$1.25e+03$	$1.34e+03$	$5.95e+04$	$5.00e-03$	$2.80e-02$	$8.08e+00$	5.24	*Yes*
120	1682-31-1	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$4.82e+02$	$3.99e+03$	$8.66e+03$	$1.68e-04$	$6.00e-03$	$1.73e+01$	5.96	*Yes*
121	1715-40-8	`BrCC1CC2(Cl)C(=C(Cl)C1(Cl)C2(Cl)Cl)Cl`		$7.05e+02$	$3.63e+03$	$1.75e+05$	$8.80e-05$	$6.00e-03$	$2.35e+00$	6.015	*Yes*
122	1735-48-4	`FC(F)(F)C(F)(C(F)(C(F)(F)F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$7.38e+03$	$9.63e+03$	$3.89e+06$	$2.99e-05$	$1.33e-03$	$1.00e+06$	6.54	*Yes*
123	1765-48-6	`FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)O`		$1.06e+03$	$5.62e+01$	$1.14e+06$	$1.01e-03$	$4.10e-02$	$2.06e+01$	6.21	*Yes*
124	1825-19-0	`CSc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.67e+02$	$3.20e+03$	$2.74e+04$	$1.83e-04$	$7.00e-03$	$8.80e+00$	5.82	*Yes*
125	1825-21-4	`COc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.74e+02$	$1.18e+04$	$4.15e+05$	$8.40e-04$	$2.60e-02$	$9.77e+00$	5.375	*No*
126	1919-45-5	`Clc1ccc(cc1)Oc1nc(Oc2ccc(Cl)cc2)nc(n1)Oc1ccc(Cl)cc1`		$3.18e+02$	$1.46e+03$	$6.91e+06$	$3.00e-04$	$1.30e-05$	$2.44e+00$	7.9	*No*

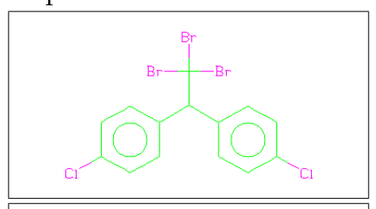
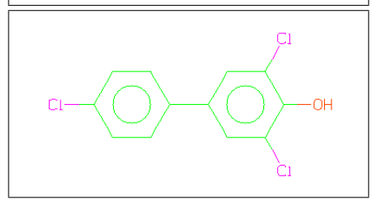
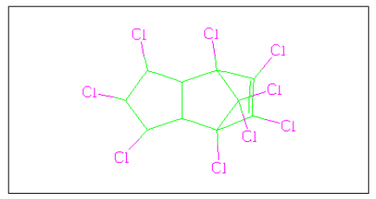
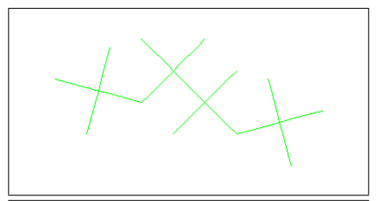
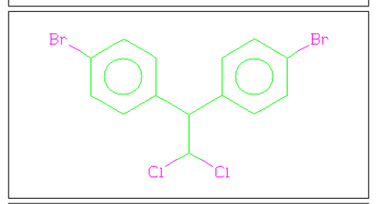
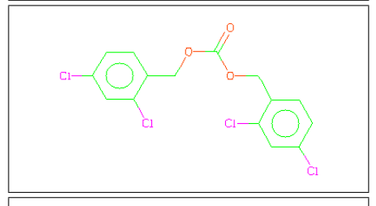
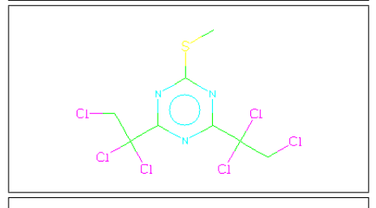
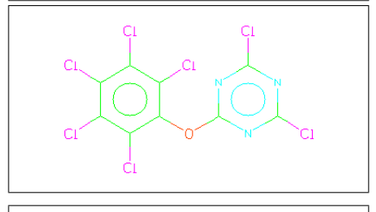
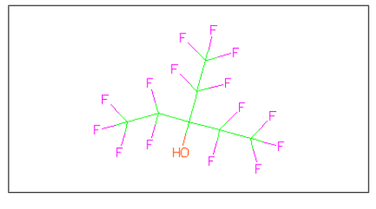
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
127	1940-20-1	`Oc1c(Cc2c(O)c(Cl)cc(Cl)c2Cl)cc(Cl)c(Cl)c1Cl`		$3.42e+02$	$1.72e+04$	$1.12e+03$	$1.83e-03$	$2.10e-02$	$4.91e+00$	6.92	*No*
128	2043-52-9	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.48e+03$	$9.48e+03$	$7.19e+05$	$3.58e-06$	$1.99e-04$	$1.73e+01$	7.3	*Yes*
129	2043-53-0	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.59e+03$	$4.46e+03$	$1.56e+06$	$5.14e-07$	$3.49e-05$	$1.73e+01$	7.97	*Yes*
130	2043-54-1	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$7.95e+03$	$9.84e+02$	$7.21e+05$	$1.04e-08$	$1.05e-06$	$1.73e+01$	9.31	*Yes*
131	2043-57-4	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.45e+02$	$1.10e+04$	$1.14e+05$	$2.47e-05$	$1.13e-03$	$1.73e+01$	6.63	*Yes*
132	2051-24-3	`Clc1c(Cl)c(Cl)c(Cl)c(c1Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.18e+03$	$1.46e+04$	$6.81e+06$	$5.09e-10$	$6.69e-08$	$5.89e+02$	9.235	*Yes*
133	2058-94-8	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.77e+03$	$5.62e+01$	$5.65e+06$	$1.65e-04$	$8.00e-03$	$2.06e+01$	6.82	*Yes*
134	2136-95-0	`Clc1c(Cl)c(C(Cl)Cl)c(Cl)c(Cl)c1Cl`		$3.51e+02$	$5.70e+03$	$6.25e+04$	$1.63e-05$	$5.20e-02$	$3.37e+01$	6.2	*No*
135	2172-49-8	`Clc1ccc(cc1)C(CC(=O)Cl)(c1ccc(Cl)cc1)c1ccc(Cl)cc1`		$1.92e+02$	$8.36e+03$	$2.29e+06$	$2.00e-03$	$5.50e-02$	$2.13e+00$	6.45	*Yes*

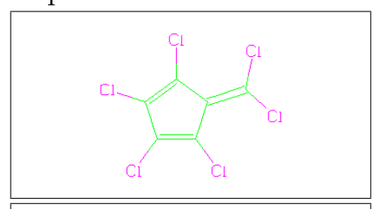
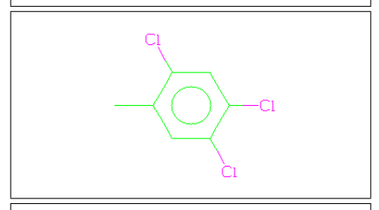
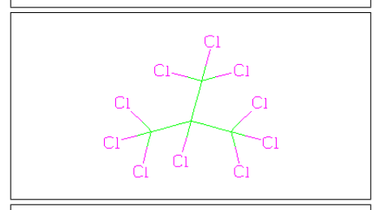
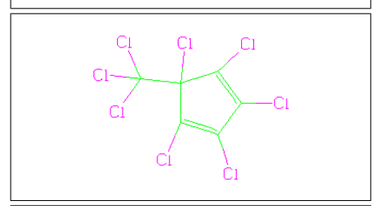
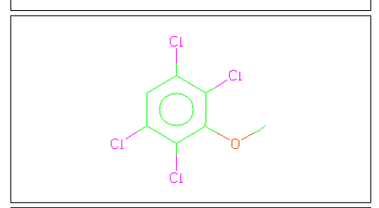
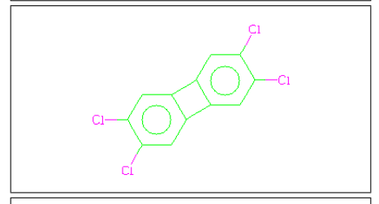
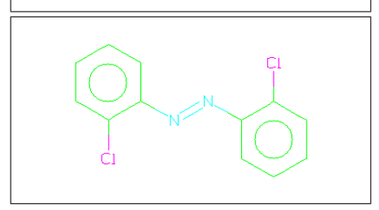
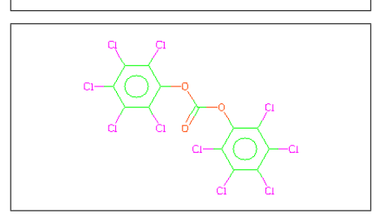
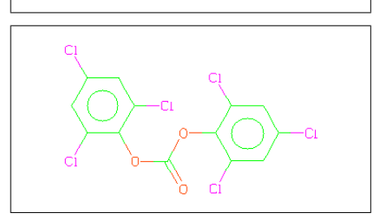
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
136	2172-51-2	N#CCC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)c1ccc(Cl)cc1		$1.92e+02$	$1.37e+04$	$5.87e+06$	$1.30e-05$	$6.19e-04$	$2.08e+00$	6.78	*Yes*
137	2227-13-6	Clc1ccc(cc1)Sc1cc(Cl)c(Cl)cc1Cl		$1.30e+02$	$1.58e+04$	$2.71e+06$	$8.21e-06$	$4.02e-04$	$2.42e+00$	6.87	*Yes*
138	2227-17-0	ClC1=C(Cl)C(Cl)(C(=C1Cl)Cl)C1(Cl)C(=C(Cl)C(=C1Cl)Cl)Cl		$2.33e+03$	$2.77e+03$	$5.69e+06$	$1.19e-07$	$1.86e-05$	$1.36e+01$	8.39	*Yes*
139	2234-13-1	Clc1c(Cl)c(Cl)c(Cl)c2c1c(Cl)c(Cl)c(Cl)c2Cl		$7.40e+02$	$1.89e+03$	$2.22e+05$	$1.23e-07$	$9.27e-06$	$2.78e+02$	8.415	*Yes*
140	2274-74-0	Clc1ccc(SN=Nc2cc(Cl)c(Cl)cc2Cl)cc1		$1.44e+02$	$1.00e+01$	$1.57e+06$	$1.65e-05$	$6.60e-05$	$2.83e+00$	6.67	*No*
141	2482-68-0	ClC(=C(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$7.37e+02$	$3.06e+03$	$1.89e+05$	$2.08e-04$	$1.30e-02$	$3.82e+00$	5.79	*No*
142	2550-75-6	ClCC1C(CCl)C2(Cl)C(=C(Cl)C1(Cl)C2(Cl)Cl)Cl		$1.37e+03$	$1.25e+04$	$3.79e+06$	$1.55e-05$	$1.32e-03$	$2.24e+00$	6.71	*No*
143	2642-80-0	ClCC(c1ccc(Cl)cc1)c1ccc(Cl)cc1		$8.40e+01$	$2.65e+03$	$1.20e+05$	$2.57e-04$	$9.00e-03$	$2.41e+00$	5.69	*No*
144	2888-15-5	Clc1cc(Cl)c(Cl)cc1Cc1cc(Cl)c(Cl)cc1Cl		$3.68e+02$	$4.92e+03$	$4.28e+06$	$4.37e-07$	$2.89e-05$	$6.60e+00$	7.88	*Yes*

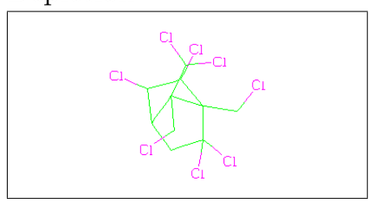
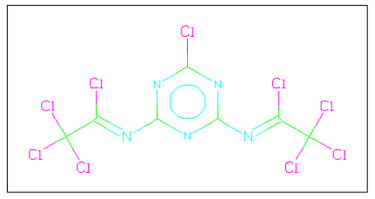
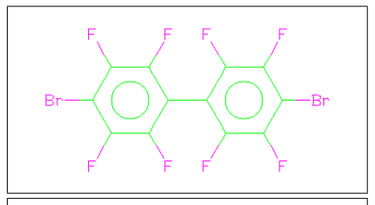
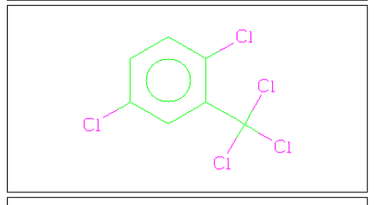
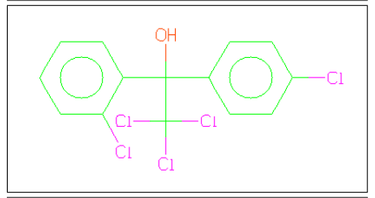
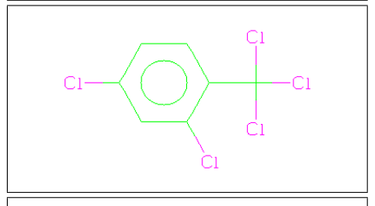
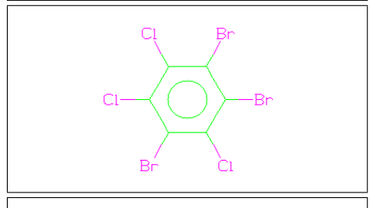
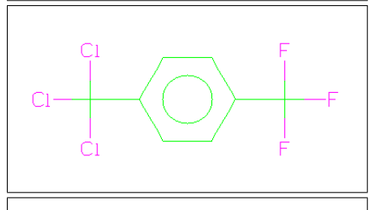
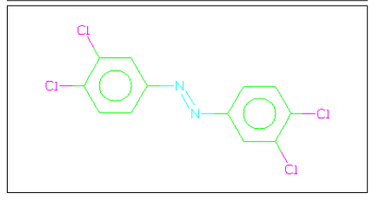
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
145	2990-17-2	`Brc1ccc(cc1)C(c1ccc(Br)cc1)C(Cl)(Cl)Cl`		$3.18e+02$	$9.64e+03$	$4.37e+06$	$3.17e-06$	$1.76e-04$	$3.46e+00$	7.29	*No*
146	3010-80-8	`Clc1ccc(cc1)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1`		$1.52e+02$	$7.79e+03$	$2.17e+06$	$4.00e-03$	$3.00e-03$	$2.11e+00$	6.31	*Yes*
147	3021-63-4	`FC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$2.26e+04$	$4.93e+03$	$1.07e+07$	$6.32e-07$	$4.17e-05$	$1.00e+06$	7.88	*No*
148	3050-42-8	`ClC(=C(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl)Cl`		$7.37e+02$	$4.03e+03$	$3.39e+05$	$1.20e-04$	$8.00e-03$	$1.38e+01$	5.97	*No*
149	3095-73-6	`BrCc1c(CBr)c(CBr)c(CBr)c(CBr)c1CBr`		$7.55e+01$	$9.09e+03$	$2.98e+00$	$2.33e-06$	$1.50e-02$	$4.96e+00$	7.34	*Yes*
150	3114-54-3	`Clc1ccc(cc1)c1nc(nc(n1)c1ccc(Cl)cc1)c1ccc(Cl)cc1`		$1.95e+02$	$3.94e+03$	$3.53e+06$	$1.51e-03$	$1.36e-04$	$3.56e+00$	7.02	*No*
151	3182-02-3	`Clc1ccc(NC2=NN(C(=O)C2)c2c(Cl)cc(Cl)cc2Cl)c(Cl)c1`		$3.44e+02$	$4.80e+03$	$1.25e+05$	$1.98e-05$	$7.94e-05$	$2.35e+00$	6.08	*Yes*
152	3194-55-6	`BrC1CCC(Br)C(Br)CCC(Br)C(Br)CCC1Br`		$7.73e+01$	$5.76e+03$	$3.87e+05$	$1.15e-06$	$7.27e-05$	$2.13e+00$	7.74	*Yes*
153	3268-87-9	`Clc1c2Oc3c(Oc2c(Cl)c(Cl)c1Cl)c(Cl)c(Cl)c(Cl)c3Cl`		$1.12e+03$	$2.12e+03$	$3.67e+04$	$3.98e-09$	$4.25e-07$	$1.97e+02$	8.85	*No*

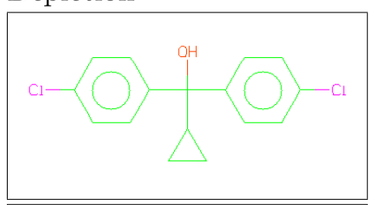
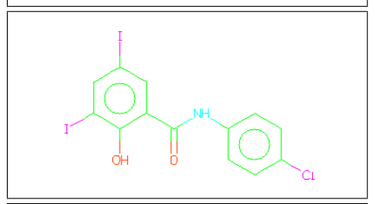
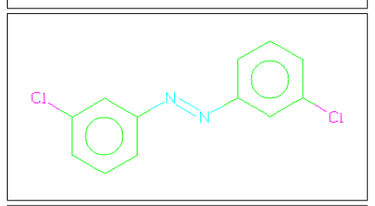
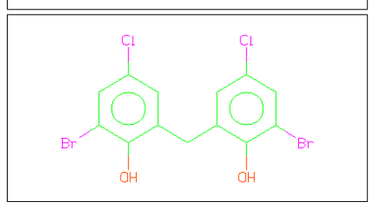
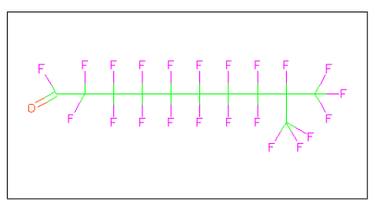
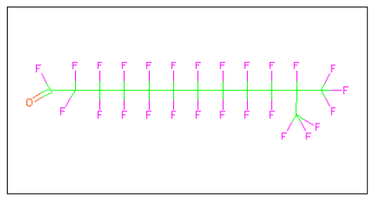
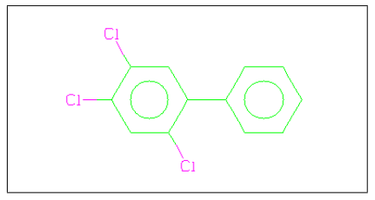
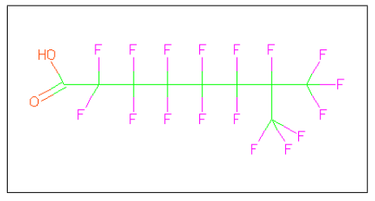
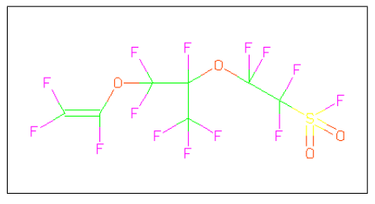
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
154	3330-16-3	FC(OC(F)(F)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)F)C(F)(F)F		$3.22e+04$	$5.24e+03$	$9.86e+06$	$4.45e-04$	$6.00e-03$	$4.13e+03$	7.83	*No*
155	3486-08-6	FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$2.24e+03$	$9.09e+03$	$2.85e+05$	$3.79e-05$	$1.67e-03$	$1.00e+06$	6.5	*Yes*
156	3513-93-7	ClC(Cl)C1CC2(Cl)C(=C(Cl)C1(Cl)C2(Cl)Cl)Cl		$1.30e+03$	$5.91e+03$	$1.03e+06$	$6.53e-05$	$5.00e-03$	$2.41e+00$	6.22	*No*
157	3563-45-9	Clc1ccc(cc1)C(Cl)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl		$5.65e+02$	$1.31e+04$	$7.19e+06$	$2.99e-06$	$1.70e-02$	$3.25e+00$	7.01	*No*
158	3584-22-3	Cc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$9.38e+02$	$1.13e+03$	$1.41e+05$	$3.76e-05$	$3.00e-03$	$2.49e+00$	5.92	*No*
159	3599-72-2	O=N(=O)c1cccc(c1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$1.24e+03$	$3.74e+02$	$6.63e+03$	$2.12e-04$	$2.50e-02$	$3.58e+01$	5.19	*No*
160	3599-80-2	Clc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)c1ccccc1		$2.94e+02$	$1.06e+03$	$2.40e+05$	$3.92e-05$	$3.00e-03$	$2.44e+00$	5.87	*No*
161	3658-57-9	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)Cl		$1.30e+03$	$1.00e+01$	$6.42e+05$	$1.79e-03$	$6.70e-02$	$2.06e+01$	5.98	*Yes*
162	3712-60-5	Clc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$1.27e+03$	$1.31e+03$	$4.41e+05$	$3.16e-05$	$2.00e-03$	$1.08e+01$	6.01	*No*

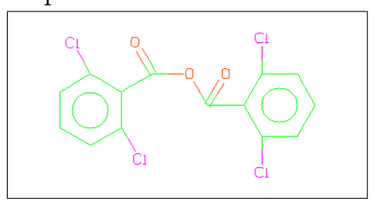
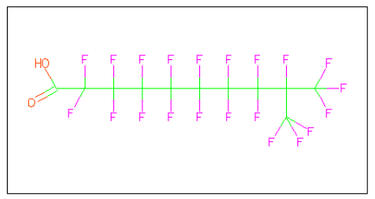
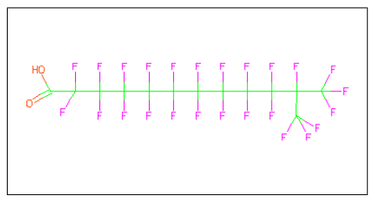
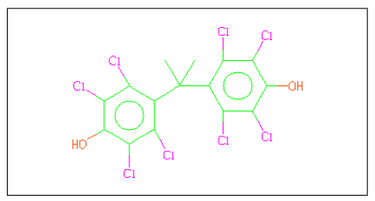
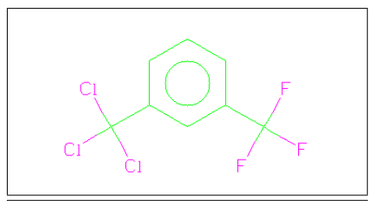
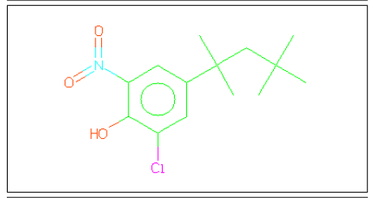
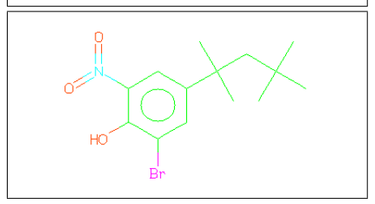
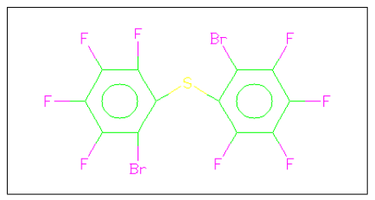
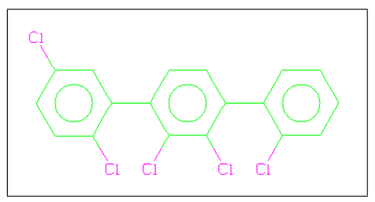
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
163	3734-49-4	`ClC1C2C(CC1(Cl)Cl)C1(Cl)C(=C(Cl)C2(Cl)C1(Cl)Cl)Cl`		$3.21e+03$	$5.72e+03$	$1.31e+06$	$4.23e-06$	$4.28e-04$	$2.28e+00$	6.69	*No*
164	3820-68-6	`Clc1ccc(OP(=O)(Oc2ccc(Cl)cc2Cl)Oc2ccc(Cl)cc2Cl)c(Cl)c1`		$4.54e+02$	$3.40e+02$	$2.84e+06$	$4.63e-08$	$5.80e-04$	$5.03e+00$	8.57	*No*
165	3871-31-6	`Clc1ccc(cc1)OP(=O)(Oc1ccc(Cl)cc1)Oc1ccc(Cl)cc1`		$1.04e+02$	$1.66e+03$	$1.42e+06$	$3.00e-03$	$1.60e-02$	$3.38e+00$	6.63	*Yes*
166	3883-86-1	`Fc1c(F)cc(F)c(F)c1c1c(F)c(F)cc(F)c1F`		$7.99e+03$	$6.16e+03$	$4.40e+04$	$7.36e-04$	$2.30e-02$	$4.52e+01$	5.36	*Yes*
167	3972-13-2	`Ic1ccc(cc1)C(c1ccc(I)cc1)C(Cl)(Cl)Cl`		$3.32e+02$	$5.16e+03$	$8.57e+05$	$7.13e-07$	$4.66e-05$	$3.31e+00$	7.84	*No*
168	4019-40-3	`Clc1ccc(cc1)NC(=O)c1cc(Cl)cc(c2ccc(Cl)cc2)c1O`		$1.17e+02$	$1.91e+04$	$2.29e+03$	$2.37e-04$	$4.57e-04$	$2.08e+00$	6.99	*No*
169	4074-25-3	`O=N(=O)c1c(cc(cc1C(C)(C)C)C(C)(C)C)C(C)(C)C`		$1.10e+02$	$7.24e+03$	$3.38e+05$	$9.64e-07$	$5.76e-05$	$2.60e+00$	7.54	*Yes*
170	4089-58-1	`FC(=O)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F)C(F)(F)F`		$2.46e+03$	$2.60e+03$	$5.03e+04$	$8.00e-03$	$2.74e-01$	$1.00e+06$	5.68	*Yes*
171	4329-07-1	`Clc1ccc(cc1)C(c1cccc(Cl)c1)C(Cl)(Cl)Cl`		$2.89e+02$	$1.41e+04$	$3.77e+06$	$1.12e-05$	$5.39e-04$	$2.12e+00$	6.79	*No*

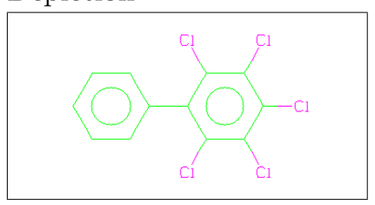
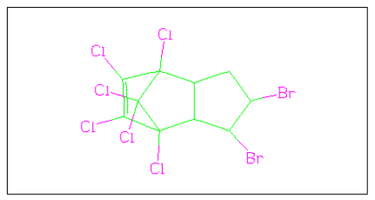
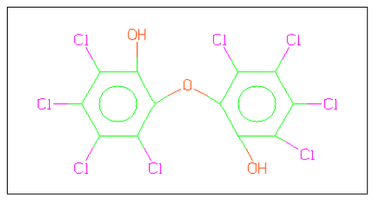
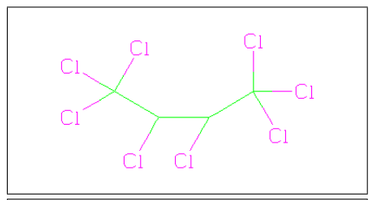
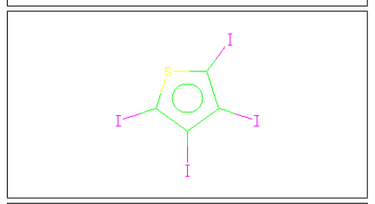
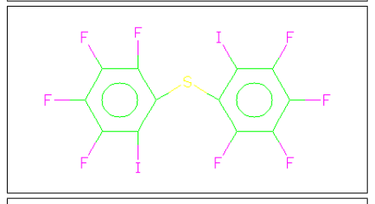
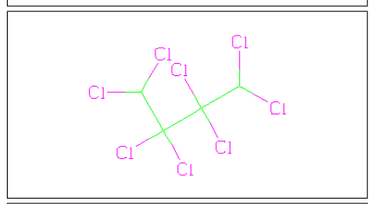
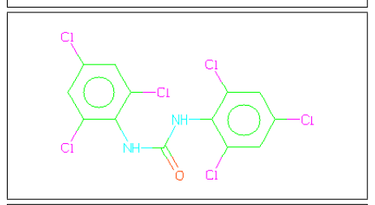
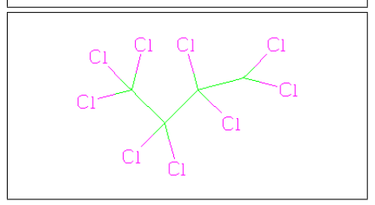
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
172	4399-08-0	`Clc1ccc(cc1)C(c1ccc(Cl)cc1)C(Br)(Br)Br`		$1.68e+02$	$1.24e+04$	$9.85e+05$	$6.85e-06$	$3.55e-04$	$3.11e+00$	7.06	*No*
173	4400-06-0	`Clc1ccc(cc1)c1cc(Cl)c(O)c(Cl)c1`		$6.77e+01$	$1.27e+03$	$6.47e+03$	$8.00e-03$	$1.90e-02$	$6.82e+00$	5.21	*No*
174	5103-73-1	`ClC1C(Cl)C2C(C1Cl)C1(Cl)C(=C(Cl)C2(Cl)C1(Cl)Cl)Cl`		$2.22e+03$	$7.19e+03$	$2.77e+06$	$3.91e-05$	$3.00e-03$	$2.68e+00$	6.395	*No*
175	5171-85-7	`CC(C)(C)CC(C)(C)C(C)(C)CC(C)(C)C`		$9.26e+01$	$5.68e+03$	$5.52e+05$	$3.89e-07$	$2.48e-05$	$2.38e+00$	7.75	*No*
176	5216-53-5	`Brc1ccc(cc1)C(C(Cl)Cl)c1ccc(Br)cc1`		$1.43e+02$	$7.35e+03$	$5.83e+05$	$4.79e-05$	$2.00e-03$	$2.68e+00$	6.36	*No*
177	5323-67-1	`O=C(OCc1ccc(Cl)cc1Cl)OCc1ccc(Cl)cc1Cl`		$1.61e+02$	$5.97e+03$	$1.80e+04$	$3.32e-04$	$3.10e-02$	$2.00e+00$	6.23	*No*
178	5516-48-3	`CSc1nc(nc(n1)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl`		$7.74e+02$	$8.52e+02$	$1.34e+04$	$5.52e-05$	$5.00e-03$	$7.80e+00$	5.73	*No*
179	5599-24-6	`Clc1nc(Cl)nc(n1)Oc1c(Cl)c(Cl)c(Cl)c1Cl`		$9.13e+02$	$6.27e+02$	$1.91e+04$	$2.90e-02$	$9.00e-03$	$2.49e+02$	5.53	*No*
180	6189-00-0	`FC(F)(F)C(F)(F)C(O)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$2.48e+03$	$7.65e+02$	$7.49e+03$	$4.00e-03$	$1.13e-01$	$7.64e+01$	4.88	*No*

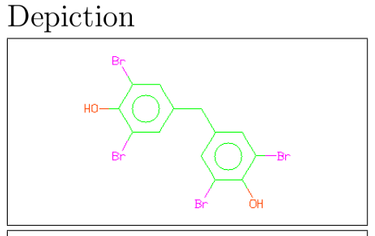
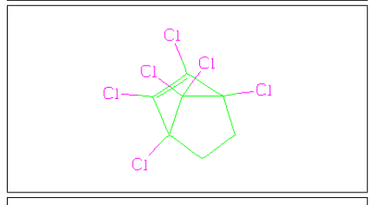
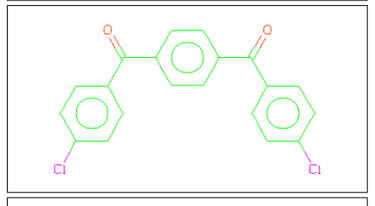
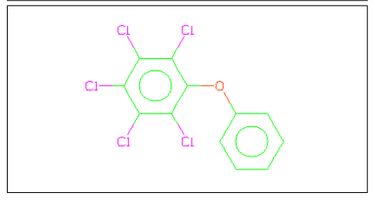
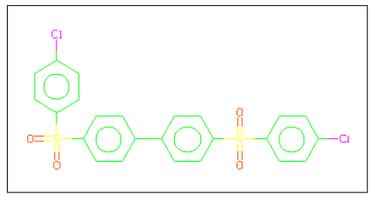
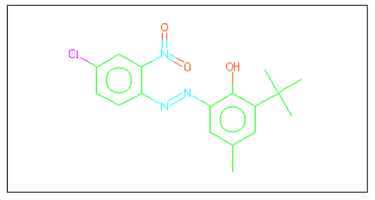
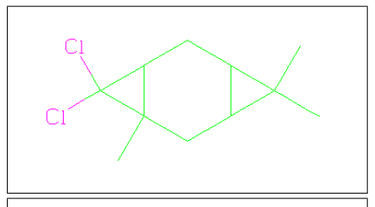
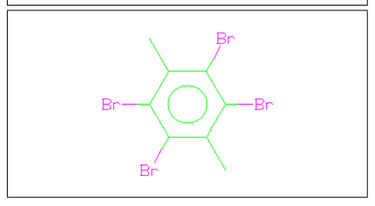
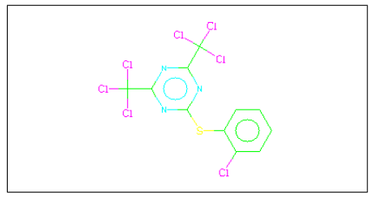
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
181	6317-25-5	`ClC(=C1C(=C(Cl)C(=C1Cl)Cl)Cl)Cl`		$1.61e+02$	$1.93e+03$	$6.62e+04$	$4.43e-04$	$2.40e-02$	$2.73e+00$	5.48	*No*
182	6639-30-1	`Clc1cc(Cl)c(Cl)cc1C`		$6.30e+01$	$5.53e+03$	$1.01e+04$	$7.00e-03$	$1.71e-01$	$2.22e+01$	4.515	*Yes*
183	6820-74-2	`ClC(C(Cl)(Cl)Cl)(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.69e+03$	$9.24e+03$	$1.24e+06$	$2.98e-05$	$1.31e-03$	$1.00e+06$	6.52	*No*
184	6928-57-0	`ClC1=C(Cl)C(Cl)(C(=C1Cl)Cl)C(Cl)(Cl)Cl`		$8.08e+02$	$5.84e+03$	$5.70e+05$	$6.20e-05$	$4.00e-03$	$2.72e+01$	6.21	*No*
185	6936-40-9	`COc1c(Cl)c(Cl)cc(Cl)c1Cl`		$1.06e+02$	$1.67e+03$	$7.55e+03$	$5.00e-03$	$1.32e-01$	$6.16e+00$	4.665	*Yes*
186	7090-41-7	`Clc1cc2c(cc1Cl)c1cc(Cl)c(Cl)cc21`		$1.14e+02$	$2.02e+04$	$2.01e+04$	$3.71e-05$	$1.55e-03$	$3.48e+01$	6.24	*No*
187	7334-33-0	`Clc1ccccc1N=Nc1ccccc1Cl`		$8.06e+01$	$1.00e+01$	$4.19e+04$	$1.18e-05$	$4.71e-05$	$9.84e+00$	5.4	*Yes*
188	7497-08-7	`O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.75e+03$	$6.68e+02$	$5.49e+05$	$6.80e-10$	$8.24e-05$	$1.26e+02$	9.65	*No*
189	7497-11-2	`O=C(Oc1c(Cl)cc(Cl)cc1Cl)Oc1c(Cl)cc(Cl)cc1Cl`		$3.86e+02$	$1.22e+04$	$3.34e+06$	$1.31e-05$	$7.00e-03$	$1.07e+01$	7.07	*Yes*

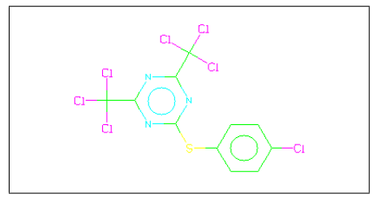
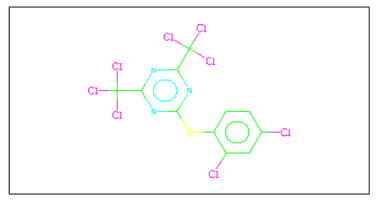
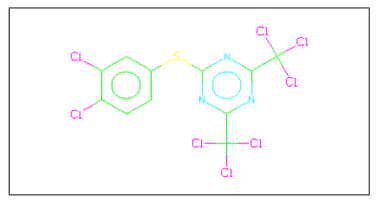
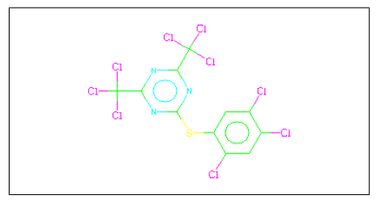
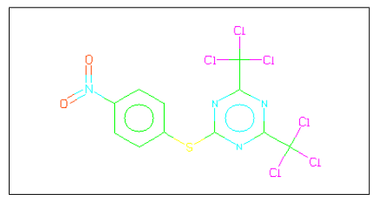
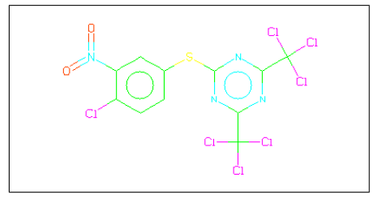
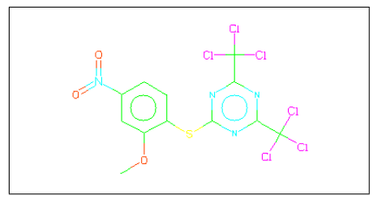
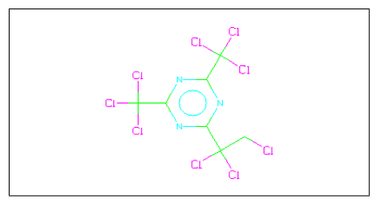
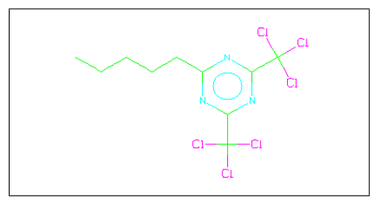
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
190	8001-35-2	`ClCC12C(Cl)C(Cl)C(CC1(Cl)Cl)C2(CCl)C(Cl)Cl`		$1.46e+03$	$7.99e+03$	$2.78e+05$	$1.31e-05$	$7.20e-06$	$4.75e+00$	6.285	*Yes*
191	10243-83-1	`Clc1nc(nc(n1)N=C(Cl)C(Cl)(Cl)Cl)N=C(Cl)C(Cl)(Cl)Cl`		$2.79e+03$	$2.73e+02$	$1.19e+04$	$9.70e-02$	$4.80e-02$	$2.03e+02$	4.98	*No*
192	10386-84-2	`Fc1c(Br)c(F)c(F)c(c1F)c1c(F)c(F)c(Br)c(F)c1F`		$2.35e+04$	$4.38e+04$	$2.77e+06$	$5.06e-06$	$2.69e-04$	$1.55e+02$	7.14	*Yes*
193	10541-71-6	`Clc1ccc(Cl)c(c1)C(Cl)(Cl)Cl`		$1.79e+02$	$1.22e+03$	$1.20e+04$	$1.29e-04$	$7.30e-02$	$1.46e+02$	5.18	*Yes*
194	10606-46-9	`Clc1ccc(cc1)C(O)(c1cccc1Cl)C(Cl)(Cl)Cl`		$3.90e+02$	$3.16e+03$	$3.03e+05$	$9.00e-03$	$8.00e-03$	$3.12e+00$	5.81	*No*
195	13014-18-1	`Clc1ccc(c(Cl)c1)C(Cl)(Cl)Cl`		$1.79e+02$	$1.22e+03$	$1.20e+04$	$1.29e-04$	$7.30e-02$	$6.05e+01$	5.18	*Yes*
196	13075-01-9	`Brc1c(Cl)c(Cl)c(Br)c(Br)c1Cl`		$2.64e+02$	$1.05e+04$	$1.59e+05$	$2.42e-05$	$1.09e-03$	$7.34e+02$	6.6	*No*
197	13947-96-1	`FC(F)(F)c1ccc(cc1)C(Cl)(Cl)Cl`		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.98e+02$	4.86	*Yes*
198	14047-09-7	`Clc1ccc(N=Nc2ccc(Cl)c(Cl)c2)cc1Cl`		$2.15e+02$	$1.00e+01$	$2.06e+06$	$1.50e-05$	$6.00e-05$	$3.37e+01$	6.69	*No*

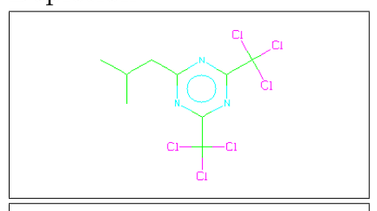
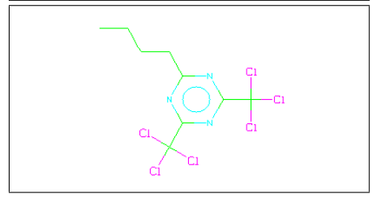
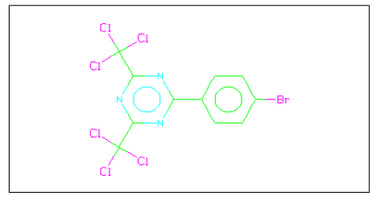
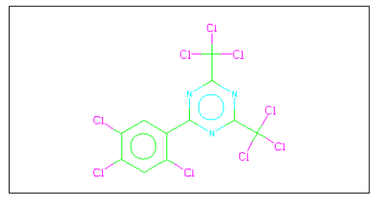
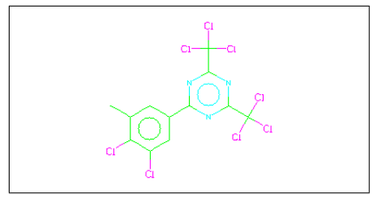
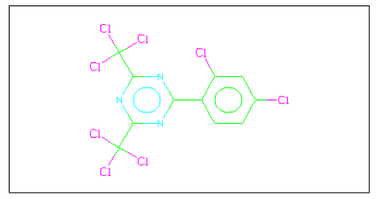
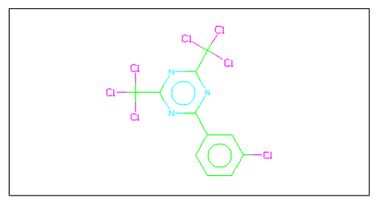
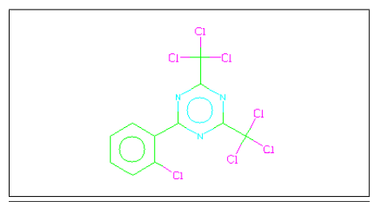
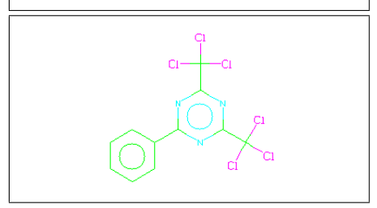
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
199	14088-71-2	`Clc1ccc(cc1)C(O)(C1CC1)c1ccc(Cl)cc1`		$8.12e+01$	$1.98e+03$	$2.77e+04$	$1.90e-02$	$2.10e-02$	$2.88e+00$	5.375	*Yes*
200	14437-46-8	`Clc1ccc(cc1)NC(=O)c1cc(I)cc(I)c1O`		$1.01e+02$	$6.42e+03$	$1.21e+02$	$8.69e-04$	$3.00e-03$	$2.67e+00$	6.28	*No*
201	15426-14-9	`Clc1cccc(N=Nc2cccc(Cl)c2)c1`		$8.06e+01$	$1.00e+01$	$4.19e+04$	$1.18e-05$	$4.71e-05$	$2.37e+01$	5.4	*No*
202	15435-29-7	`Clc1cc(Cc2cc(Cl)cc(Br)c2O)c(O)c(Br)c1`		$1.41e+02$	$5.10e+03$	$2.77e+02$	$9.00e-03$	$1.01e-01$	$2.57e+00$	6.12	*Yes*
203	15720-98-6	`FC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$8.86e+03$	$5.19e+03$	$1.51e+06$	$5.00e-03$	$1.31e-01$	$1.00e+06$	6.14	*Yes*
204	15811-52-6	`FC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$2.72e+04$	$7.80e+03$	$1.10e+07$	$7.68e-04$	$1.20e-02$	$1.00e+06$	7.47	*Yes*
205	15862-07-4	`Clc1cc(Cl)c(Cl)cc1c1ccccc1`		$6.75e+01$	$1.07e+04$	$3.28e+05$	$2.33e-04$	$8.00e-03$	$8.37e+00$	5.75	*No*
206	15899-31-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.52e+03$	$1.00e+01$	$2.85e+05$	$4.00e-03$	$1.54e-01$	$2.06e+01$	5.67	*Yes*
207	16090-14-5	`FC(=C(F)F)OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F`		$5.41e+02$	$6.08e+03$	$4.53e+05$	$1.71e-03$	$9.00e-03$	$8.08e+00$	6.24	*Yes*

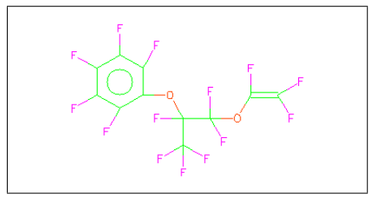
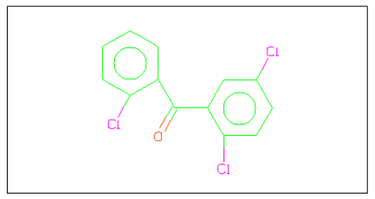
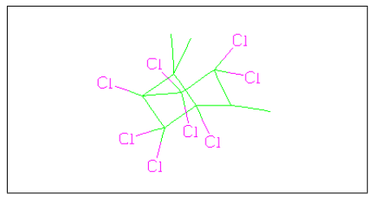
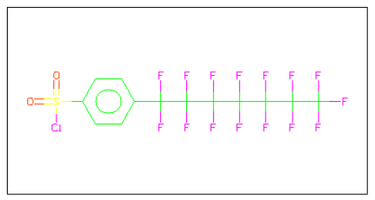
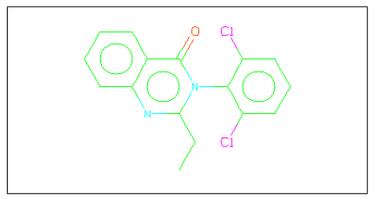
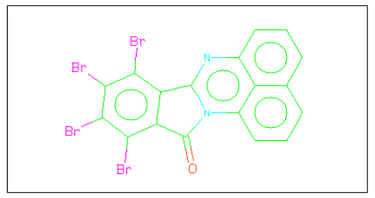
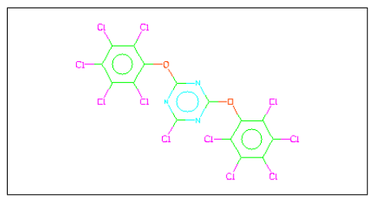
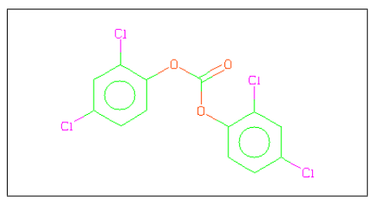
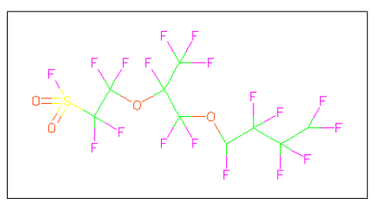
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
208	16442-10-7	`Clc1cccc(Cl)c1C(=O)OC(=O)c1c(Cl)cccc1Cl`		$1.51e+02$	$8.08e+02$	$6.98e+03$	$4.00e-03$	$9.60e-02$	$6.08e+00$	4.91	*Yes*
209	16486-94-5	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$4.67e+03$	$5.62e+01$	$7.81e+06$	$9.37e-05$	$5.00e-03$	$2.06e+01$	7.01	*Yes*
210	16486-96-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.43e+04$	$1.00e+01$	$7.82e+06$	$1.90e-06$	$1.44e-04$	$2.06e+01$	8.35	*Yes*
211	16669-42-4	`Oc1c(Cl)c(Cl)c(c(Cl)c1Cl)C(C)(C)c1c(Cl)c(Cl)c(O)c(Cl)c1Cl`		$1.29e+03$	$1.75e+03$	$2.32e+04$	$5.60e-05$	$6.85e-04$	$2.68e+00$	8.8	*No*
212	16766-90-8	`FC(F)(F)c1cccc(c1)C(Cl)(Cl)Cl`		$2.13e+02$	$7.46e+02$	$7.06e+03$	$2.70e-04$	$8.80e-02$	$1.49e+02$	4.86	*Yes*
213	17199-21-2	`Clc1cc(cc(N(=O)=O)c1O)C(C)(C)CC(C)(C)C`		$9.70e+01$	$6.82e+03$	$8.43e+02$	$4.00e-03$	$1.58e-03$	$4.16e+00$	6.32	*No*
214	17199-22-3	`Brc1cc(cc(N(=O)=O)c1O)C(C)(C)CC(C)(C)C`		$1.02e+02$	$9.91e+03$	$7.63e+02$	$3.00e-03$	$1.04e-03$	$4.19e+00$	6.56	*No*
215	17728-68-6	`Fc1c(Sc2c(F)c(F)c(F)c(F)c2Br)c(Br)c(F)c(F)c1F`		$2.66e+04$	$6.22e+03$	$1.07e+06$	$1.07e-06$	$6.67e-05$	$8.30e+00$	7.67	*No*
216	17760-93-9	`Clc1ccc(Cl)c(c1)c1ccc(c2ccccc2Cl)c(Cl)c1Cl`		$2.51e+02$	$7.17e+03$	$4.11e+06$	$3.44e-08$	$2.94e-06$	$9.12e+00$	8.74	*No*

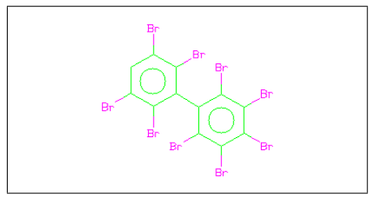
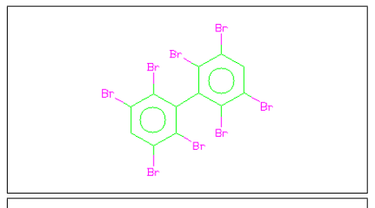
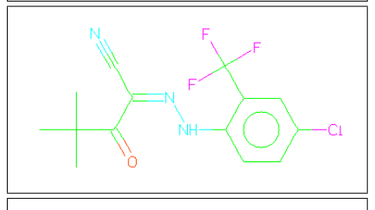
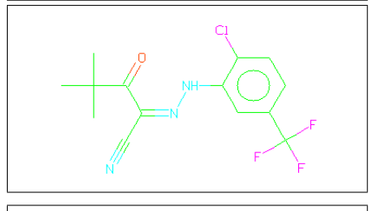
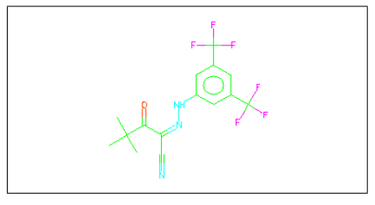
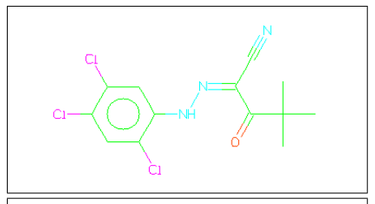
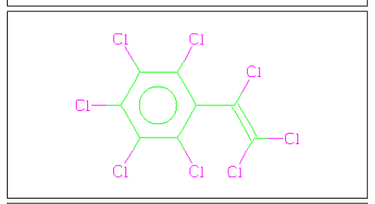
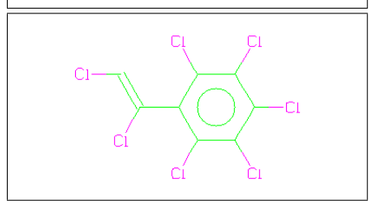
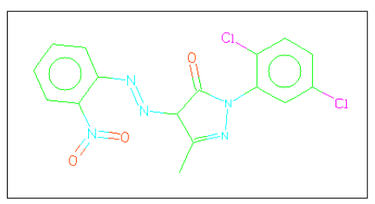
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
217	18259-05-7	`Clc1c(c2ccccc2)c(Cl)c(Cl)c(Cl)c1Cl`		$1.80e+02$	$6.00e+04$	$1.33e+06$	$5.91e-06$	$2.99e-04$	$1.55e+01$	6.865	*No*
218	18300-04-4	`BrC1CC2C(C1Br)C1(Cl)C(=C(Cl)C2(Cl)C1(Cl)Cl)Cl`		$1.00e+03$	$8.23e+03$	$8.87e+05$	$4.41e-05$	$3.00e-03$	$2.06e+00$	6.44	*Yes*
219	18632-75-2	`Oc1c(Oc2c(O)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$8.94e+02$	$8.42e+03$	$4.86e+03$	$8.27e-04$	$1.00e-02$	$7.30e+00$	7.41	*No*
220	18791-19-0	`ClC(C(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$7.43e+02$	$1.64e+03$	$1.11e+04$	$7.80e-04$	$2.50e-02$	$2.92e+02$	5.38	*No*
221	19259-11-1	`Ic1sc(I)c(I)c1I`		$1.16e+02$	$8.79e+03$	$7.40e+01$	$4.00e-03$	$7.20e-02$	$2.37e+01$	6.48	*Yes*
222	19638-37-0	`Fc1c(Sc2c(F)c(F)c(F)c(F)c2I)c(I)c(F)c(F)c1F`		$2.78e+04$	$3.33e+03$	$6.72e+04$	$2.38e-07$	$1.74e-05$	$7.21e+00$	8.23	*No*
223	20338-26-5	`ClC(Cl)C(Cl)(Cl)C(Cl)(Cl)C(Cl)Cl`		$7.43e+02$	$1.64e+03$	$1.11e+04$	$7.80e-04$	$2.50e-02$	$7.64e+01$	5.38	*No*
224	20632-35-3	`O=C(Nc1c(Cl)cc(Cl)cc1Cl)Nc1c(Cl)cc(Cl)cc1Cl`		$3.83e+02$	$1.50e+04$	$6.76e+03$	$3.19e-04$	$8.00e-03$	$4.81e+00$	6.84	*No*
225	21483-62-5	`ClC(Cl)C(Cl)(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl`		$1.66e+03$	$6.66e+03$	$4.07e+05$	$5.25e-05$	$2.00e-03$	$1.53e+02$	6.3	*No*

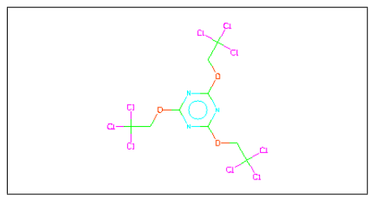
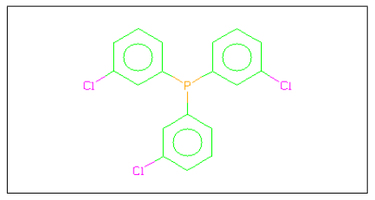
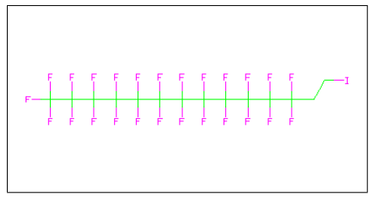
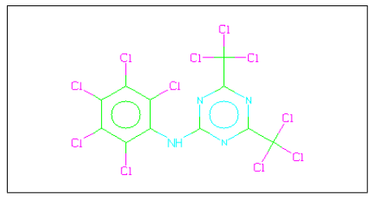
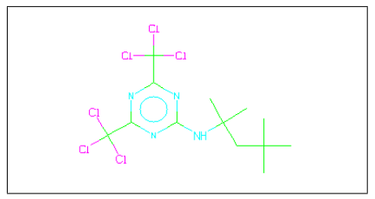
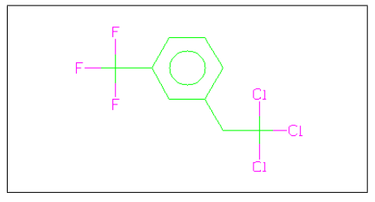
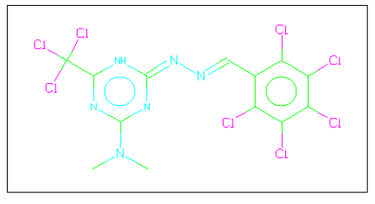
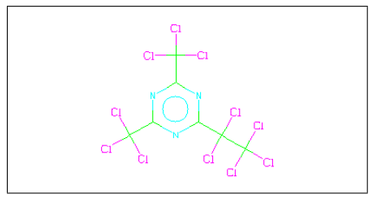
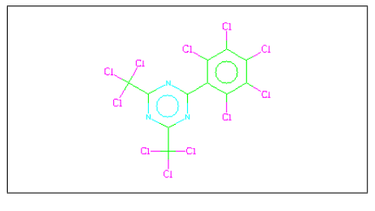
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
226	21825-03-6	`Brc1cc(Cc2cc(Br)c(O)c(Br)c2)cc(Br)c1O`		$1.55e+02$	$1.08e+04$	$1.83e+02$	$4.00e-03$	$4.90e-02$	$2.77e+00$	6.62	*Yes*
227	22039-38-9	`ClC1=C(Cl)C2(Cl)CCC1(Cl)C2(Cl)Cl`		$5.19e+02$	$1.62e+03$	$3.16e+04$	$6.62e-04$	$3.50e-02$	$2.50e+00$	5.37	*No*
228	22198-42-1	`Clc1ccc(cc1)C(=O)c1ccc(cc1)C(=O)c1ccc(Cl)cc1`		$7.71e+01$	$5.89e+02$	$8.43e+04$	$4.36e-04$	$1.50e-02$	$3.29e+00$	5.59	*Yes*
229	22274-42-6	`Clc1c(Oc2ccccc2)c(Cl)c(Cl)c(Cl)c1Cl`		$2.12e+02$	$7.41e+03$	$8.17e+04$	$3.26e-05$	$1.40e-03$	$6.75e+00$	6.4	*No*
230	22287-56-5	`Clc1ccc(cc1)S(=O)(=O)c1ccc(cc1)c1ccc(cc1)S(=O)(=O)c1ccc(Cl)cc1`		$1.26e+02$	$6.41e+03$	$9.34e+05$	$7.75e-05$	$3.00e-03$	$5.26e+00$	6.27	*Yes*
231	22617-04-5	`Clc1ccc(N=Nc2cc(C)cc(c2O)C(C)(C)C)c(c1)N(=O)=O`		$1.63e+02$	$6.00e+00$	$1.11e+04$	$1.63e-05$	$5.99e-05$	$5.64e+00$	7.83	*Yes*
232	22819-70-1	`CC1(C)C2CC3(C)C(CC12)C3(Cl)Cl`		$1.14e+02$	$4.66e+03$	$4.38e+04$	$6.36e-05$	$2.00e-03$	$7.93e+00$	6.07	*Yes*
233	23488-38-2	`Cc1c(Br)c(Br)c(C)c(Br)c1Br`		$1.50e+02$	$1.13e+04$	$8.26e+03$	$2.09e-05$	$9.58e-04$	$2.25e+01$	6.65	*Yes*
234	24478-06-6	`Clc1ccccc1Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.44e+03$	$2.95e+03$	$1.39e+06$	$1.01e-05$	$5.76e-04$	$2.91e+00$	6.55	*No*

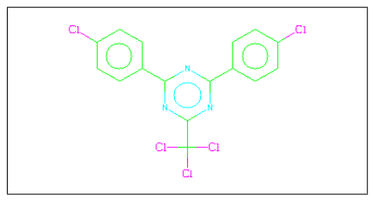
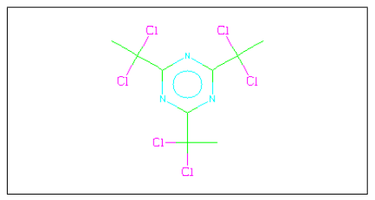
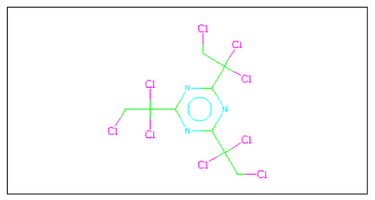
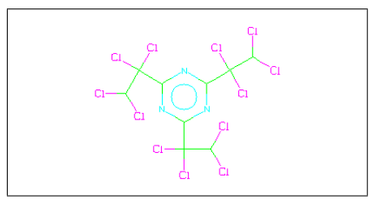
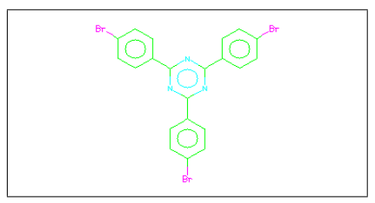
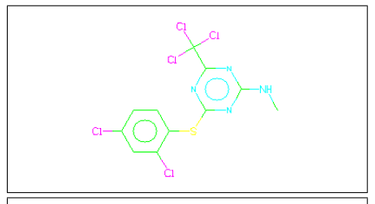
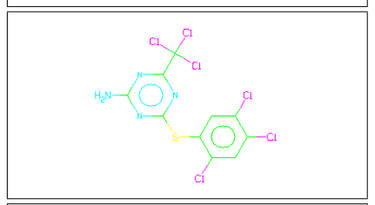
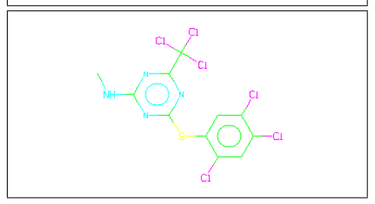
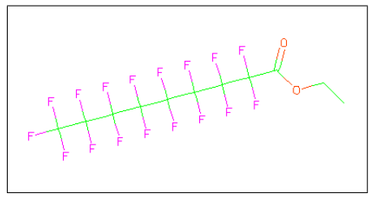
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
235	24478-08-8	`Clc1ccc(cc1)Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.44e+03$	$3.56e+03$	$1.79e+06$	$1.01e-05$	$5.76e-04$	$2.91e+00$	6.61	*No*
236	24478-09-9	`Clc1ccc(Sc2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c1`		$2.36e+03$	$3.26e+03$	$3.95e+06$	$2.51e-06$	$1.02e-04$	$9.95e+00$	7.19	*No*
237	24478-10-2	`Clc1ccc(Sc2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)cc1Cl`		$2.36e+03$	$3.26e+03$	$3.95e+06$	$2.51e-06$	$1.02e-04$	$4.14e+00$	7.19	*No*
238	24478-11-3	`Clc1cc(Cl)c(Cl)cc1Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.85e+03$	$1.58e+03$	$5.11e+06$	$6.22e-07$	$1.79e-05$	$1.41e+01$	7.84	*No*
239	24478-14-6	`O=N(=O)c1ccc(cc1)Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.41e+03$	$8.40e+02$	$2.24e+04$	$6.78e-05$	$6.00e-03$	$6.80e+00$	5.72	*No*
240	24478-15-7	`O=N(=O)c1cc(ccc1Cl)Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.30e+03$	$2.24e+03$	$1.90e+05$	$1.68e-05$	$1.05e-03$	$3.30e+01$	6.36	*No*
241	24478-16-8	`COc1cc(ccc1Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)N(=O)=O`		$1.75e+03$	$9.50e+02$	$1.33e+04$	$6.00e-05$	$5.00e-03$	$4.88e+00$	5.8	*No*
242	24481-33-2	`ClCC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.44e+03$	$1.28e+03$	$1.65e+05$	$3.43e-05$	$3.00e-03$	$1.13e+02$	6	*No*
243	24481-37-6	`CCCCCc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$5.17e+02$	$1.54e+03$	$2.84e+04$	$2.26e-05$	$1.62e-03$	$2.02e+00$	6.12	*No*

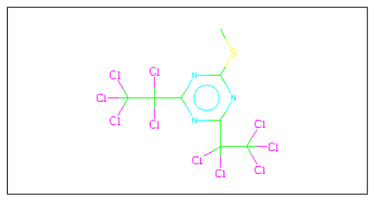
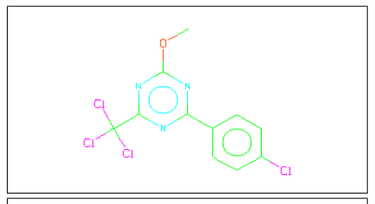
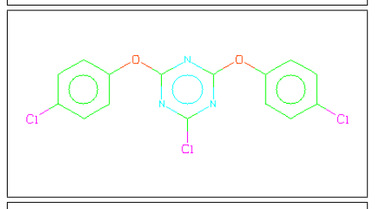
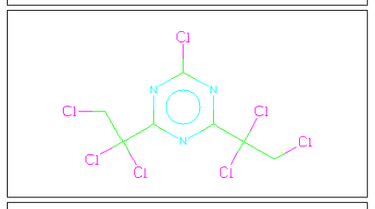
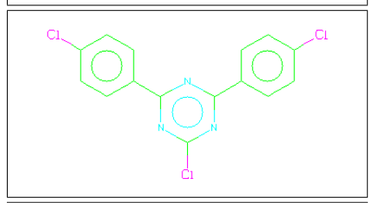
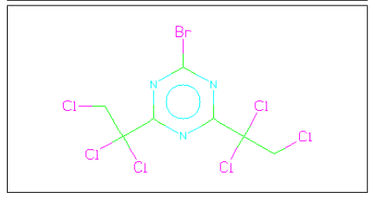
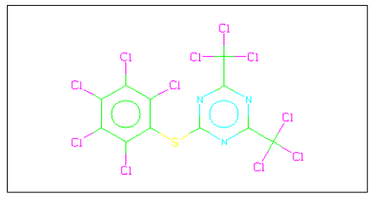
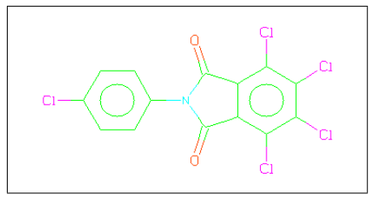
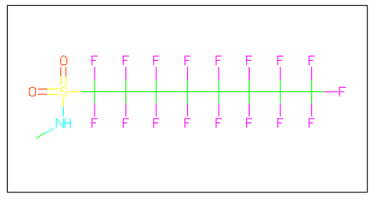
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
244	24481-40-1	`CC(C)Cc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$8.23e+02$	$6.51e+02$	$5.30e+03$	$7.87e-05$	$8.00e-03$	$2.76e+00$	5.55	*No*
245	24481-41-2	`CCCCc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$4.90e+02$	$7.28e+02$	$7.12e+03$	$6.66e-05$	$6.00e-03$	$2.75e+00$	5.63	*No*
246	24481-49-0	`Brc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.34e+03$	$1.90e+03$	$6.58e+05$	$2.00e-05$	$1.33e-03$	$1.10e+01$	6.26	*No*
247	24481-50-3	`Clc1cc(Cl)c(Cl)cc1c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.40e+03$	$2.35e+03$	$1.41e+06$	$1.54e-05$	$9.50e-04$	$5.23e+01$	6.4	*No*
248	24481-51-4	`Cc1cc(cc(Cl)c1Cl)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.50e+03$	$3.21e+03$	$2.89e+06$	$2.35e-06$	$9.44e-05$	$5.47e+00$	7.21	*No*
249	24481-52-5	`Clc1ccc(c(Cl)c1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.08e+03$	$8.82e+02$	$2.07e+05$	$6.20e-05$	$5.00e-03$	$1.55e+01$	5.75	*No*
250	24481-54-7	`Clc1cccc(c1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.27e+03$	$1.31e+03$	$4.41e+05$	$3.16e-05$	$2.00e-03$	$4.48e+00$	6.01	*No*
251	24481-55-8	`Clc1ccccc1c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.27e+03$	$3.31e+02$	$2.02e+04$	$2.48e-04$	$3.00e-02$	$1.08e+01$	5.11	*No*
252	24504-22-1	`ClC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)Cl)c1ccccc1`		$7.51e+02$	$4.93e+02$	$5.22e+03$	$1.26e-04$	$1.30e-02$	$3.15e+00$	5.37	*No*

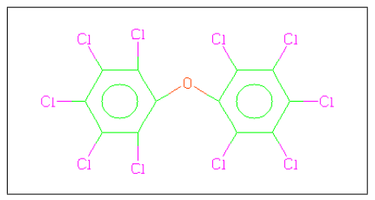
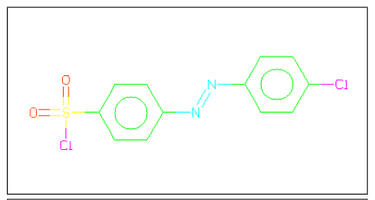
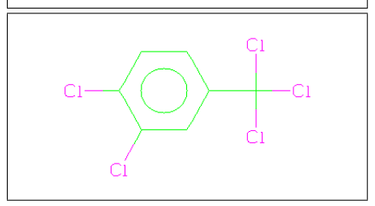
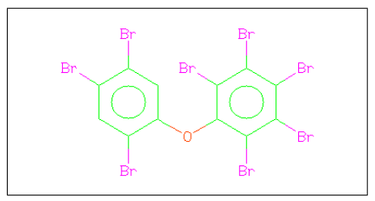
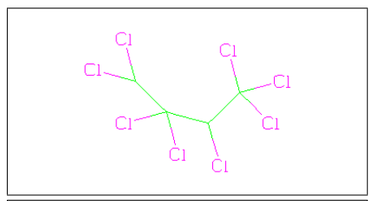
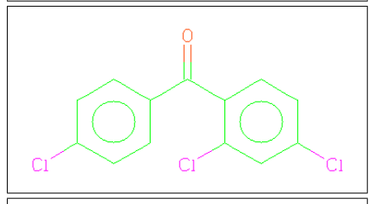
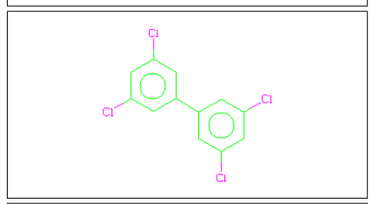
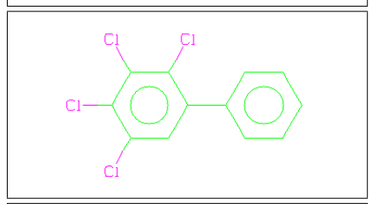
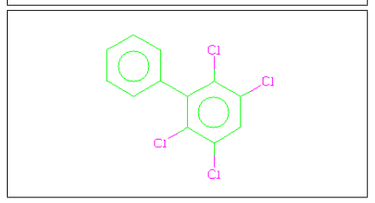
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
253	24520-19-2	FC(=C(F)F)OC(F)(F)C(F)(Oc1c(F)c(F)c(F)c(F)c1F)C(F)(F)F		$9.10e+03$	$2.49e+03$	$1.26e+05$	$3.00e-03$	$1.70e-02$	$4.08e+00$	5.65	*Yes*
254	25187-06-8	Clc1ccc(Cl)c(c1)C(=O)c1ccccc1Cl		$8.13e+01$	$2.72e+02$	$8.77e+03$	$1.65e-03$	$4.70e-02$	$6.62e+00$	5.08	*Yes*
255	25267-15-6	CC1C(Cl)(Cl)C(Cl)(Cl)C2(Cl)C(C)(C)C1(Cl)C2(Cl)Cl		$4.41e+03$	$3.88e+03$	$4.51e+06$	$2.56e-07$	$1.80e-05$	$1.08e+01$	8.09	*No*
256	25444-35-3	ClS(=O)(=O)c1ccc(cc1)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.60e+03$	$3.37e+03$	$3.93e+06$	$2.14e-04$	$2.00e-03$	$1.16e+01$	8.22	*Yes*
257	25509-07-3	CCc1nc2ccccc2c(=O)n1c1c(Cl)cccc1Cl		$6.82e+01$	$2.17e+03$	$2.57e+04$	$1.59e-03$	$6.30e-02$	$3.06e+00$	5.56	*Yes*
258	26011-65-4	Brc1c(Br)c(Br)c2c(c1Br)C(=O)n1c2nc2cccc3cccc1c23		$2.17e+02$	$5.04e+03$	$5.38e+01$	$4.91e-04$	$1.30e-02$	$4.04e+00$	6.12	*Yes*
259	26396-34-9	Clc1nc(nc(n1)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl		$1.03e+04$	$2.95e+02$	$1.02e+06$	$2.55e-05$	$3.40e-07$	$1.07e+02$	9.32	*No*
260	26496-99-1	Clc1ccc(OC(=O)Oc2ccc(Cl)cc2Cl)c(Cl)c1		$1.44e+02$	$3.05e+03$	$1.38e+05$	*NA*	$5.84e-02$	$7.55e+00$	5.78	*Yes*
261	26654-97-7	FC(OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F)C(F)(F)C(F)(F)C(F)F		$1.67e+03$	$6.34e+03$	$2.57e+06$	$4.84e-04$	$7.00e-03$	$1.10e+04$	7.66	*No*

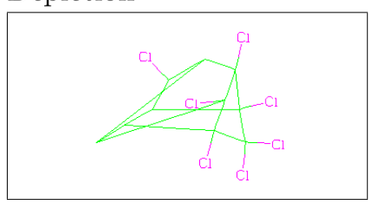
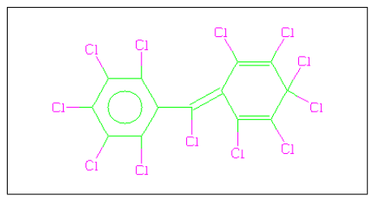
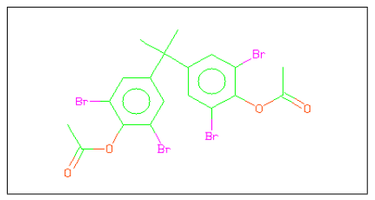
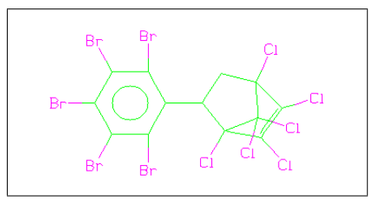
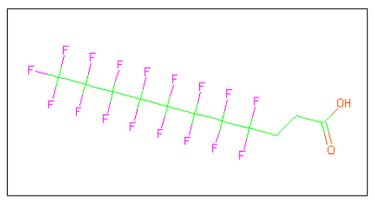
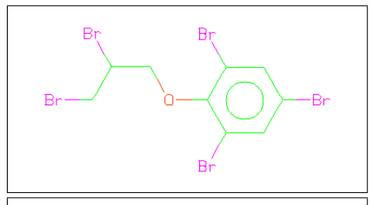
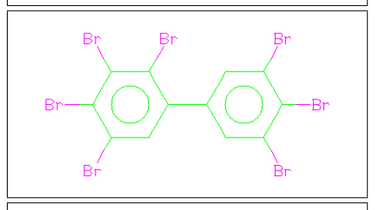
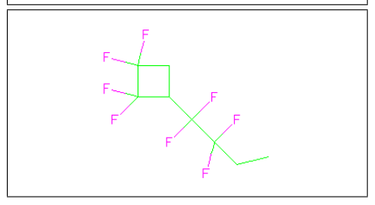
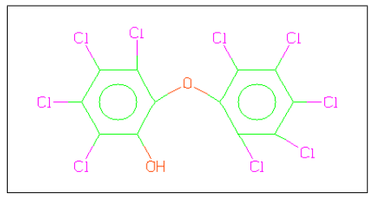
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
262	27753-52-2	`Brc1c(Br)c(Br)c(c(Br)c1Br)c1c(Br)c(Br)cc(Br)c1Br`		$2.06e+03$	$2.37e+02$	$5.37e+03$	$7.62e-12$	$1.59e-09$	$4.39e+02$	11.77	*Yes*
263	27858-07-7	`Brc1c(Br)cc(Br)c(Br)c1c1c(Br)c(Br)cc(Br)c1Br`		$1.20e+03$	$7.62e+03$	$2.47e+04$	$1.03e-10$	$1.66e-08$	$2.48e+02$	8.19	*Yes*
264	28317-94-4	`N#CC(=NNc1ccc(Cl)cc1C(F)(F)F)C(=O)C(C)(C)C`		$1.92e+02$	$2.56e+03$	$1.75e+04$	$1.55e-05$	$6.22e-05$	$2.61e+00$	5.99	*No*
265	28343-25-1	`N#CC(=NNc1cc(ccc1Cl)C(F)(F)F)C(=O)C(C)(C)C`		$1.92e+02$	$1.48e+03$	$6.38e+03$	$1.55e-05$	$6.22e-05$	$3.08e+00$	5.81	*No*
266	28343-27-3	`N#CC(=NNc1cc(cc(c1)C(F)(F)F)C(F)(F)F)C(=O)C(C)(C)C`		$3.73e+02$	$1.80e+03$	$1.78e+04$	$1.71e-05$	$6.84e-05$	$4.17e+00$	6.035	*No*
267	28343-28-4	`N#CC(=NNc1cc(Cl)c(Cl)cc1Cl)C(=O)C(C)(C)C`		$1.62e+02$	$3.42e+03$	$1.55e+04$	$1.56e-05$	$6.23e-05$	$2.58e+00$	6.25	*No*
268	29082-74-4	`ClC(=C(Cl)Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$5.67e+02$	$2.20e+04$	$3.45e+06$	$1.57e-06$	$1.75e-04$	$9.97e+00$	7.46	*No*
269	29086-38-2	`ClC=C(Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$3.68e+02$	$1.84e+04$	$2.92e+06$	$6.25e-06$	$5.86e-04$	$2.75e+00$	6.97	*No*
270	29330-49-2	`Clc1ccc(Cl)c(c1)N1N=C(C)C(N=Nc2ccccc2N(=O)=O)C1=O`		$1.86e+02$	$1.00e+01$	$1.31e+05$	$1.84e-05$	$7.35e-05$	$2.72e+00$	6.23	*Yes*

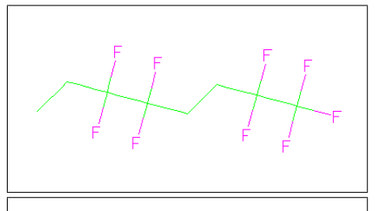
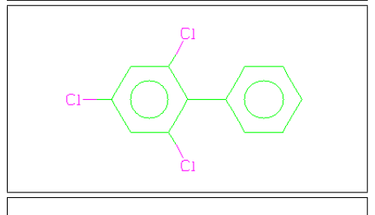
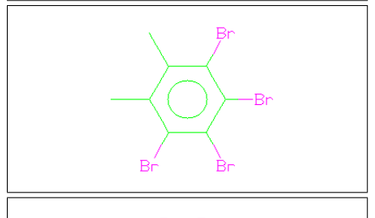
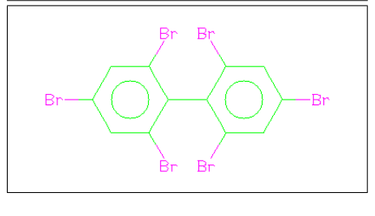
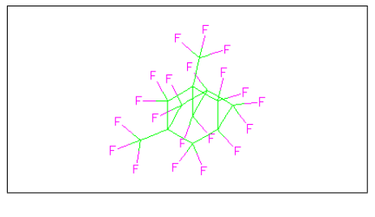
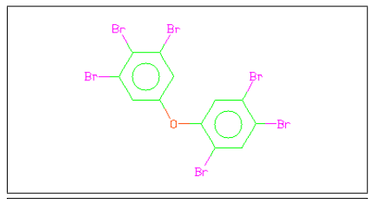
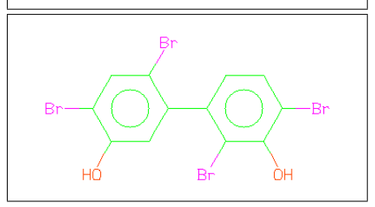
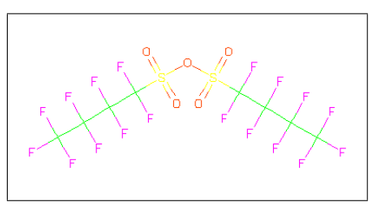
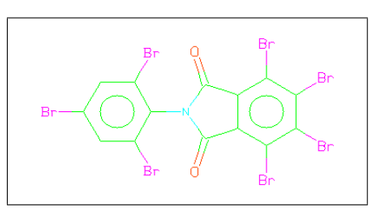
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
271	29808-66-0	`ClC(Cl)(Cl)COc1nc(OCC(Cl)(Cl)Cl)nc(OCC(Cl)(Cl)Cl)n1`		$6.23e+03$	$9.67e+02$	$9.00e+05$	$1.65e-04$	$5.29e-06$	$8.38e+00$	8.27	*No*
272	29949-85-7	`Clc1cccc(c1)P(c1cccc(Cl)c1)c1cccc(Cl)c1`		$1.06e+02$	$1.80e+04$	$8.40e+06$	$7.14e-06$	$3.58e-04$	$2.60e+00$	6.95	*Yes*
273	30046-31-2	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.44e+04$	$2.18e+02$	$7.33e+04$	$2.05e-10$	$3.08e-08$	$1.73e+01$	10.65	*Yes*
274	30356-57-1	`Clc1c(Nc2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.22e+04$	$7.60e+02$	$2.25e+06$	$1.57e-07$	$3.21e-06$	$5.90e+00$	8.48	*No*
275	30357-71-2	`CC(C)(C)CC(C)(C)Nc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.51e+03$	$2.86e+03$	$5.08e+05$	$1.74e-06$	$6.62e-05$	$4.74e+00$	7.31	*No*
276	30359-53-6	`ClC(Cl)(Cl)Cc1cccc(c1)C(F)(F)F`		$2.55e+02$	$1.57e+03$	$1.73e+04$	$7.06e-04$	$2.20e-02$	$1.34e+01$	5.35	*No*
277	30359-63-8	`CN(C)c1nc(=NN=Cc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)[nH]c(n1)C(Cl)(Cl)Cl`		$3.50e+03$	$3.35e+03$	$1.07e+04$	$2.49e-05$	$9.97e-05$	$2.33e+00$	7.17	*No*
278	30362-35-7	`ClC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.18e+04$	$3.61e+03$	$3.79e+06$	$3.24e-06$	$1.38e-04$	$1.77e+03$	7.1	*No*
279	30362-55-1	`Clc1c(c2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$9.10e+03$	$1.87e+03$	$6.48e+06$	$9.37e-07$	$2.92e-05$	$2.52e+02$	7.69	*No*

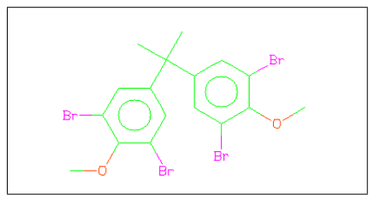
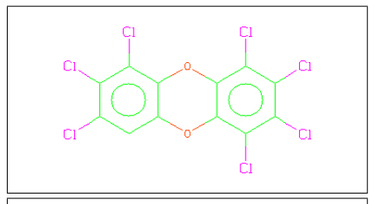
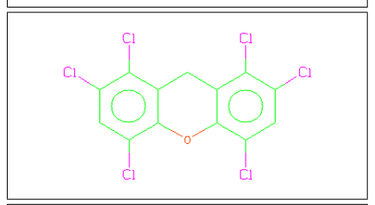
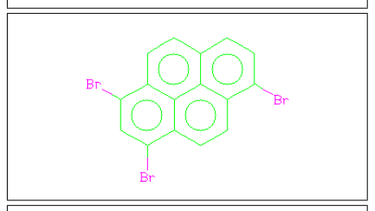
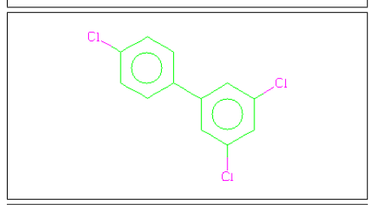
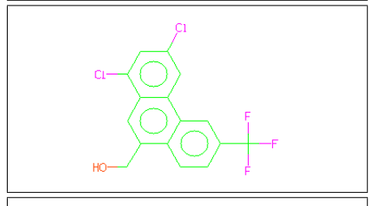
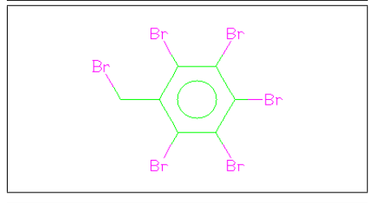
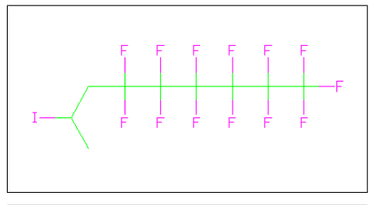
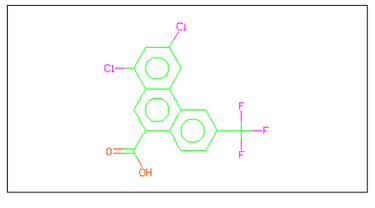
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
280	30362-65-3	`Clc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)c1ccc(Cl)cc1`		$4.99e+02$	$2.83e+03$	$4.47e+06$	$9.87e-06$	$5.70e-04$	$5.38e+00$	6.52	*No*
281	30362-74-4	`CC(Cl)(Cl)c1nc(nc(n1)C(C)(Cl)Cl)C(C)(Cl)Cl`		$1.04e+03$	$1.79e+03$	$1.53e+05$	$1.73e-05$	$1.17e-03$	$2.96e+01$	6.22	*No*
282	30362-75-5	`ClCC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl`		$3.83e+03$	$5.71e+03$	$1.64e+06$	$3.91e-06$	$1.77e-04$	$2.04e+01$	6.98	*No*
283	30362-76-6	`ClC(Cl)C(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)C(Cl)Cl)C(Cl)(Cl)C(Cl)Cl`		$1.40e+04$	$2.24e+03$	$4.28e+06$	$1.39e-06$	$4.73e-05$	$2.28e+01$	7.52	*No*
284	30363-03-2	`Brc1ccc(cc1)c1nc(nc(n1)c1ccc(Br)cc1)c1ccc(Br)cc1`		$2.25e+02$	$1.71e+03$	$2.66e+06$	$4.69e-04$	$2.29e-05$	$3.63e+00$	7.76	*No*
285	30369-61-0	`CNc1nc(Sc2ccc(Cl)cc2Cl)nc(n1)C(Cl)(Cl)Cl`		$5.95e+02$	$9.14e+02$	$1.33e+04$	$5.16e-05$	$4.00e-03$	$4.52e+00$	5.78	*No*
286	30369-62-1	`Nc1nc(Sc2cc(Cl)c(Cl)cc2Cl)nc(n1)C(Cl)(Cl)Cl`		$9.22e+02$	$1.06e+03$	$7.39e+03$	$4.34e-05$	$4.00e-03$	$1.37e+01$	5.87	*No*
287	30369-63-2	`CNc1nc(Sc2cc(Cl)c(Cl)cc2Cl)nc(n1)C(Cl)(Cl)Cl`		$9.73e+02$	$2.43e+03$	$1.07e+05$	$1.29e-05$	$7.88e-04$	$5.23e+00$	6.42	*No*
288	30377-52-7	`CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.48e+03$	$6.28e+03$	$2.62e+04$	$1.47e-03$	$4.60e-02$	$1.17e+01$	6.26	*Yes*

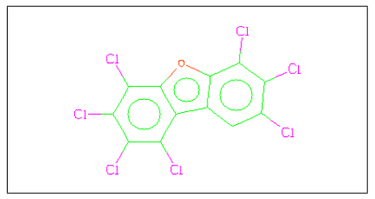
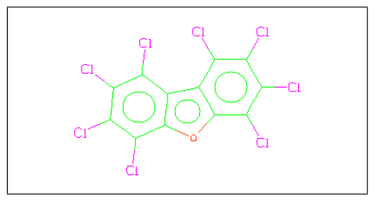
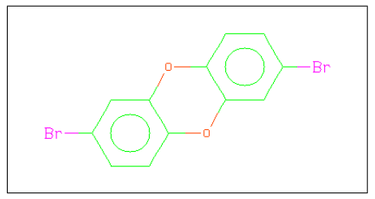
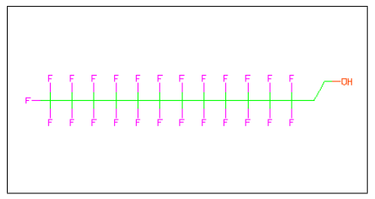
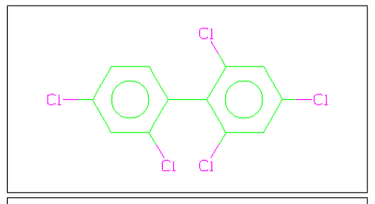
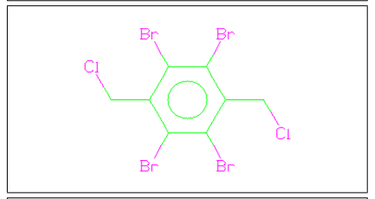
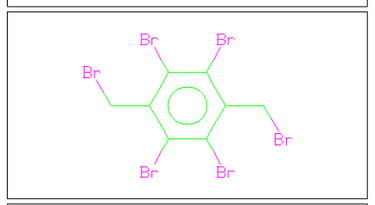
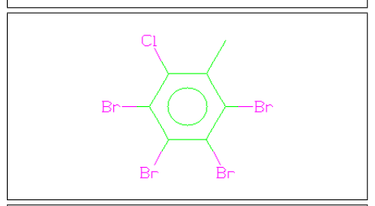
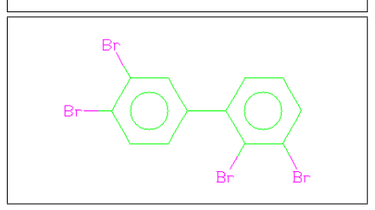
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
289	30863-02-6	`CSc1nc(nc(n1)C(Cl)(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)C(Cl)(Cl)Cl`		$9.15e+03$	$1.41e+03$	$3.67e+06$	$4.99e-07$	$1.37e-05$	$8.96e+00$	7.93	*No*
290	30863-62-8	`COc1nc(nc(n1)C(Cl)(Cl)Cl)c1ccc(Cl)cc1`		$2.83e+02$	$3.21e+02$	$5.91e+03$	$2.07e-04$	$2.50e-02$	$5.83e+00$	5.09	*No*
291	30894-78-1	`Clc1ccc(cc1)Oc1nc(Oc2ccc(Cl)cc2)nc(Cl)n1`		$2.02e+02$	$1.02e+03$	$1.46e+05$	$1.40e-02$	$3.00e-03$	$4.85e+00$	5.85	*No*
292	30894-91-8	`ClCC(Cl)(Cl)c1nc(Cl)nc(n1)C(Cl)(Cl)CCl`		$1.06e+03$	$4.00e+02$	$6.52e+03$	$1.66e-04$	$1.90e-02$	$4.45e+01$	5.23	*No*
293	30894-94-1	`Clc1ccc(cc1)c1nc(Cl)nc(n1)c1ccc(Cl)cc1`		$1.46e+02$	$4.18e+02$	$9.35e+04$	$4.00e-02$	$1.60e-02$	$6.13e+00$	5.26	*No*
294	30894-99-6	`ClCC(Cl)(Cl)c1nc(Br)nc(n1)C(Cl)(Cl)CCl`		$1.11e+03$	$5.81e+02$	$8.67e+03$	$1.06e-04$	$1.10e-02$	$4.47e+01$	5.48	*No*
295	31007-95-1	`Clc1c(Sc2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.03e+04$	$3.68e+02$	$1.42e+06$	$3.76e-08$	$5.47e-07$	$6.77e+01$	9.13	*No*
296	31039-72-2	`Clc1ccc(cc1)N1C(=O)c2c(C1=O)c(Cl)c(Cl)c(Cl)c2Cl`		$2.44e+02$	$1.31e+03$	$4.25e+04$	$3.00e-03$	$1.09e-01$	$2.93e+00$	5.23	*No*
297	31506-32-8	`CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.05e+03$	$6.34e+03$	$5.88e+05$	$9.03e-04$	$2.80e-02$	$8.46e+00$	6.27	*Yes*

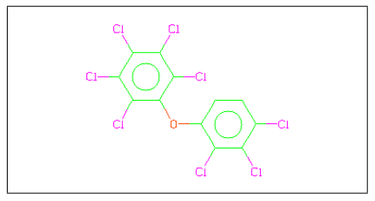
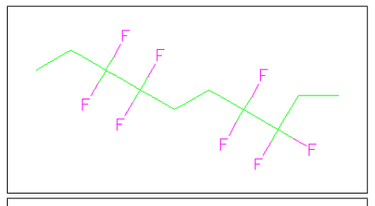
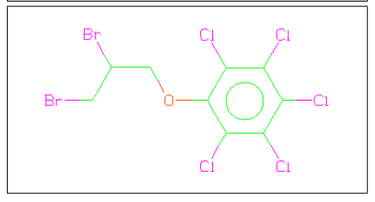
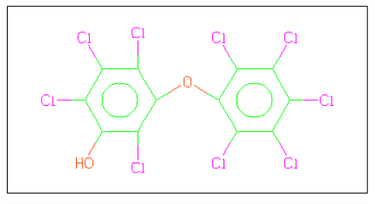
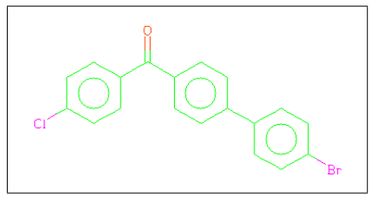
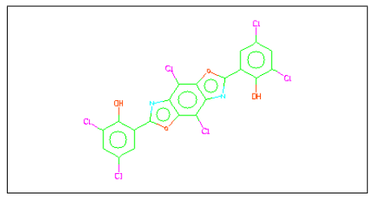
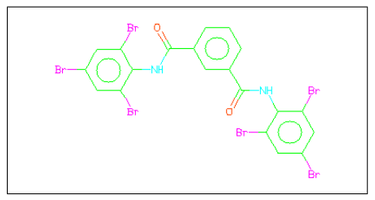
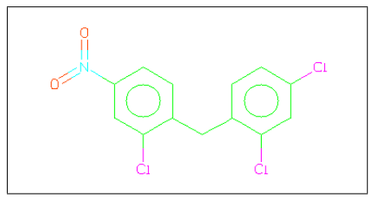
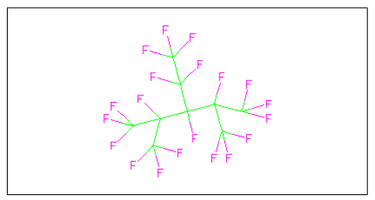
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
298	31710-30-2	`Clc1c(Cl)c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl`		$2.57e+03$	$3.59e+03$	$8.42e+05$	$2.77e-09$	$3.09e-07$	$2.19e+02$	8.905	*No*
299	31819-74-6	`Clc1ccc(N=Nc2ccc(cc2)S(=O)(=O)Cl)cc1`		$7.20e+01$	$1.00e+01$	$1.22e+04$	$1.48e-05$	$5.91e-05$	$1.51e+01$	5.7	*No*
300	31904-18-4	`Clc1ccc(cc1Cl)C(Cl)(Cl)Cl`		$1.79e+02$	$1.22e+03$	$1.20e+04$	$1.29e-04$	$7.30e-02$	$1.46e+02$	5.18	*Yes*
301	32536-52-0	`Brc1cc(Br)c(Br)cc1Oc1c(Br)c(Br)c(Br)c(Br)c1Br`		$1.41e+03$	$1.93e+03$	$3.95e+05$	$5.55e-10$	$7.58e-08$	$9.36e+01$	9.52	*Yes*
302	32694-76-1	`ClC(Cl)C(Cl)(Cl)C(Cl)C(Cl)(Cl)Cl`		$7.43e+02$	$1.64e+03$	$1.11e+04$	$7.80e-04$	$2.50e-02$	$1.29e+02$	5.38	*No*
303	33146-57-5	`Clc1ccc(cc1)C(=O)c1ccc(Cl)cc1Cl`		$8.13e+01$	$2.72e+02$	$8.77e+03$	$1.65e-03$	$4.70e-02$	$5.02e+00$	5.08	*No*
304	33284-52-5	`Clc1cc(Cl)cc(c1)c1cc(Cl)cc(Cl)c1`		$1.15e+02$	$4.05e+04$	$3.92e+06$	$3.74e-05$	$1.56e-03$	$6.08e+00$	6.47	*No*
305	33284-53-6	`Clc1cc(c2ccccc2)c(Cl)c(Cl)c1Cl`		$1.10e+02$	$2.73e+04$	$5.68e+05$	$3.74e-05$	$1.56e-03$	$1.33e+01$	6.375	*No*
306	33284-54-7	`Clc1cc(Cl)c(Cl)c(c2cccc2)c1Cl`		$1.10e+02$	$3.73e+04$	$4.66e+05$	$3.74e-05$	$1.56e-03$	$1.33e+01$	6.34	*No*

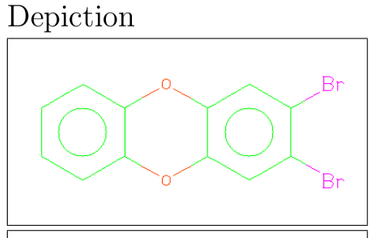
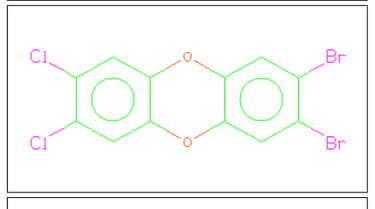
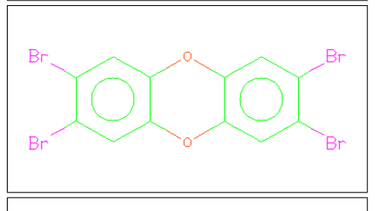
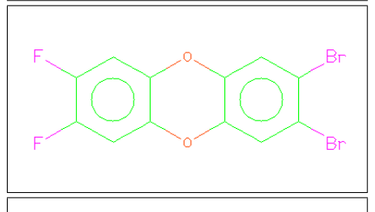
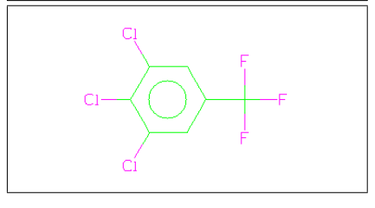
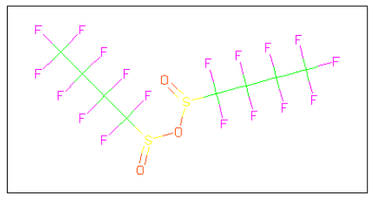
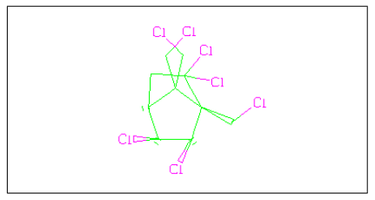
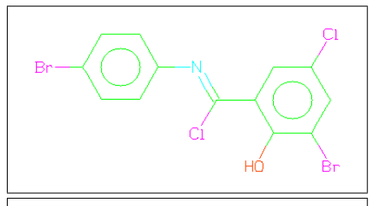
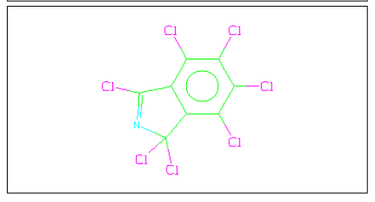
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
307	33442-83-0	`ClC1C2C3C4C1C1(Cl)C2(Cl)C(Cl)(Cl)C3(Cl)C41Cl`		$1.93e+03$	$7.73e+02$	$1.43e+04$	$4.00e-03$	$1.07e-01$	$6.77e+00$	4.88	*No*
308	33500-13-9	`Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)C(=C1C(=C(Cl)C(Cl)(Cl)C(=C1Cl)Cl)Cl)Cl`		$5.93e+03$	$1.69e+02$	$5.51e+04$	$8.49e-11$	$3.22e-08$	$2.15e+00$	10.87	*No*
309	33798-02-6	`CC(=O)Oc1c(Br)cc(cc1Br)C(C)(C)c1cc(Br)c(OC(=O)C)c(Br)c1`		$2.26e+02$	$8.89e+03$	$1.75e+02$	$6.41e-06$	$6.00e-03$	$3.66e+00$	7.36	*Yes*
310	34571-16-9	`Brc1c(Br)c(Br)c(c(Br)c1Br)C1CC2(Cl)C(=C(Cl)C1(Cl)C2(Cl)Cl)Cl`		$1.17e+04$	$8.75e+01$	$1.19e+04$	$1.96e-11$	$9.14e-09$	$2.09e+00$	11.45	*Yes*
311	34598-33-9	`OC(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.00e+03$	$5.62e+01$	$1.89e+06$	*NA*	$1.67e-02$	$7.63e+00$	6.47	*Yes*
312	35109-60-5	`BrCC(Br)COc1c(Br)cc(Br)cc1Br`		$1.39e+02$	$7.08e+03$	$2.30e+05$	$5.00e-03$	$8.50e-02$	$2.65e+00$	6.34	*Yes*
313	35194-78-6	`Brc1c(Br)cc(cc1Br)c1cc(Br)c(Br)c(Br)c1Br`		$7.00e+02$	$1.76e+03$	$2.15e+05$	$1.38e-09$	$1.71e-07$	$9.77e+01$	9.99	*No*
314	35207-97-7	`CCC(F)(F)C(F)(F)C1CC(F)(F)C1(F)F`		$1.04e+02$	$4.12e+03$	$1.67e+04$	$9.51e-05$	$4.00e-03$	$5.23e+01$	5.98	*No*
315	35245-80-8	`Oc1c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.52e+03$	$2.37e+03$	$4.69e+05$	$9.36e-05$	$1.71e-05$	$1.41e+01$	8.53	*No*

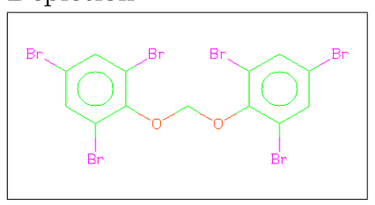
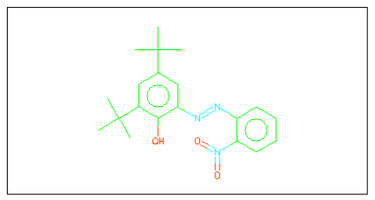
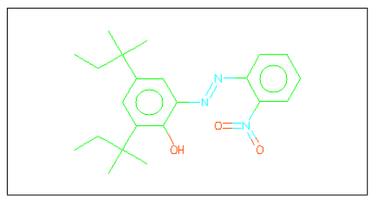
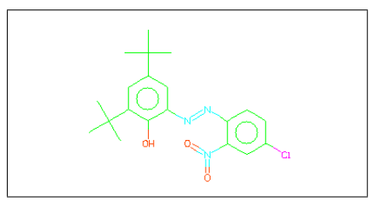
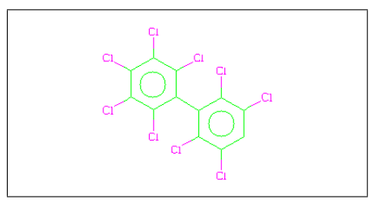
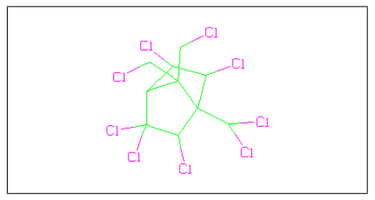
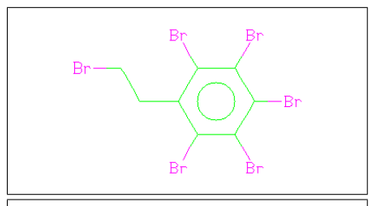
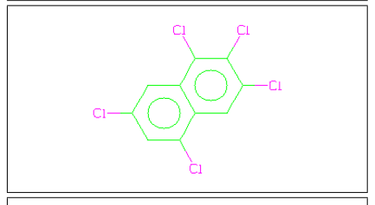
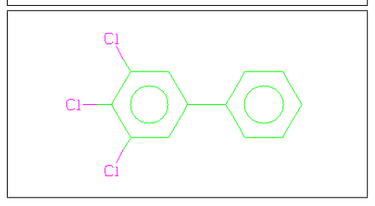
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
316	35262-54-5	`CCC(F)(F)C(F)(F)CCC(F)(F)C(F)(F)F`		$1.89e+02$	$5.00e+03$	$9.52e+04$	$6.98e-05$	$3.00e-03$	$4.74e+01$	6.11	*No*
317	35693-92-6	`Clc1cc(Cl)c(c(Cl)c1)c1ccccc1`		$6.75e+01$	$7.28e+03$	$2.67e+04$	$2.33e-04$	$8.00e-03$	$6.96e+00$	5.58	*No*
318	36059-21-9	`Cc1c(C)c(Br)c(Br)c(Br)c1Br`		$1.50e+02$	$1.13e+04$	$8.26e+03$	$2.09e-05$	$9.58e-04$	$2.25e+01$	6.65	*Yes*
319	36355-01-8	`Brc1cc(Br)c(c(Br)c1)c1c(Br)cc(Br)cc1Br`		$4.08e+02$	$3.68e+04$	$4.14e+06$	$1.83e-08$	$1.74e-06$	$3.78e+01$	7.745	*Yes*
320	36481-20-6	`FC12C(F)(F)C3(C(F)(F)F)C(F)(F)C(C(F)(F)F)(C1(F)F)C(F)(F)C(F)(C3(F)F)C2(F)F`		$1.58e+04$	$2.96e+03$	$3.96e+06$	$1.56e-07$	$1.18e-05$	$1.00e+06$	8.33	*No*
321	36483-60-0	`Brc1cc(Br)c(Br)cc1Oc1cc(Br)c(Br)c(Br)c1`		$4.81e+02$	$2.91e+03$	$8.13e+05$	$9.91e-08$	$7.98e-06$	$3.04e+01$	7.975	*Yes*
322	36511-35-0	`Brc1cc(Br)c(O)cc1c1ccc(Br)c(O)c1Br`		$1.29e+02$	$7.26e+03$	$8.14e+02$	$7.00e-03$	$7.80e-02$	$2.03e+00$	6.36	*No*
323	36913-91-4	`FC(F)(S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F`		$4.51e+03$	$3.17e+03$	$3.13e+06$	$2.08e-07$	$1.55e-05$	$1.00e+06$	8.27	*Yes*
324	37710-57-9	`Brc1cc(Br)c(c(Br)c1)N1C(=O)c2c(C1=O)c(Br)c(Br)c(Br)c2Br`		$9.13e+02$	$4.77e+03$	$1.43e+06$	$1.21e-04$	$2.00e-03$	$3.84e+01$	7.91	*No*

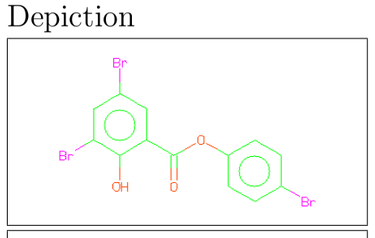
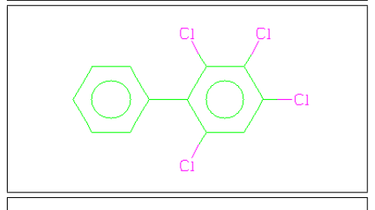
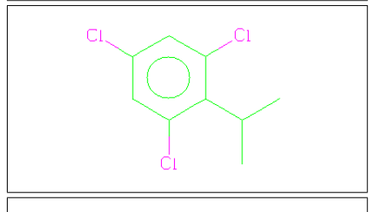
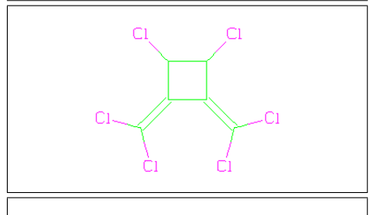
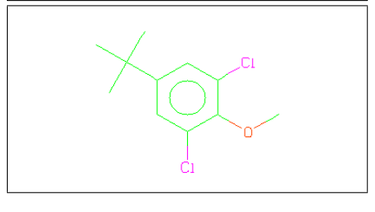
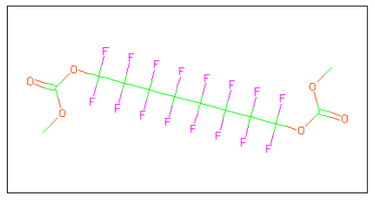
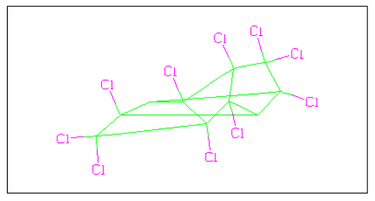
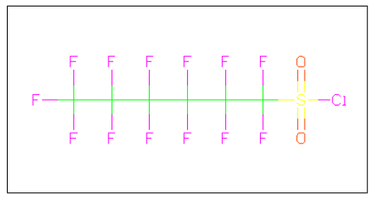
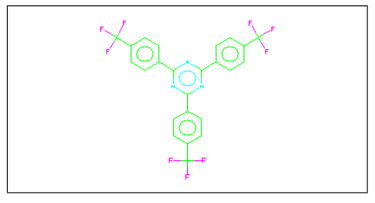
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
325	37853-61-5	`COc1c(Br)cc(cc1Br)C(C)(C)c1cc(Br)c(OC)c(Br)c1`		$3.64e+02$	$2.98e+03$	$8.60e+06$	$1.74e-07$	$1.31e-05$	$2.17e+00$	8.33	*Yes*
326	37871-00-4	`Clc1c(Cl)cc2Oc3c(Oc2c1Cl)c(Cl)c(Cl)c(Cl)c3Cl`		$6.87e+02$	$4.47e+03$	$6.69e+04$	$2.61e-08$	$2.30e-06$	$7.72e+01$	8.425	*No*
327	38178-99-3	`Clc1c(Cl)cc(Cl)c2Oc3c(Cl)cc(Cl)c(Cl)c3Cc12`		$4.30e+02$	$3.54e+03$	$1.35e+05$	$1.87e-07$	$1.35e-05$	$6.42e+00$	8.17	*No*
328	38303-36-5	`Brc1ccc2ccc3c(Br)cc(Br)c4ccc1c2c34`		$3.91e+02$	$2.60e+04$	$6.56e+02$	$1.20e-06$	$7.28e-05$	$2.79e+00$	7.6	*Yes*
329	38444-88-1	`Clc1ccc(cc1)c1cc(Cl)cc(Cl)c1`		$7.02e+01$	$1.02e+04$	$3.77e+05$	$2.33e-04$	$8.00e-03$	$5.90e+00$	5.69	*No*
330	38492-81-8	`OCc1cc2c(Cl)cc(Cl)cc2c2cc(ccc12)C(F)(F)F`		$1.27e+02$	$6.60e+03$	$6.10e+02$	$1.00e-02$	$1.00e-02$	$2.54e+00$	5.68	*Yes*
331	38521-51-6	`BrCc1c(Br)c(Br)c(Br)c(Br)c1Br`		$2.42e+02$	$9.13e+03$	$8.84e+03$	$2.09e-06$	$1.30e-02$	$3.72e+01$	7.33	*Yes*
332	38550-34-4	`CC(I)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.92e+02$	$1.26e+04$	$2.73e+05$	$7.15e-06$	$3.69e-04$	$7.95e+00$	7.05	*Yes*
333	38635-85-7	`Clc1cc(Cl)c2cc(C(=O)O)c3ccc(cc3c2c1)C(F)(F)F`		$1.52e+02$	$5.62e+01$	$8.50e+03$	$2.13e-01$	$4.50e-02$	$1.60e+01$	6.48	*Yes*

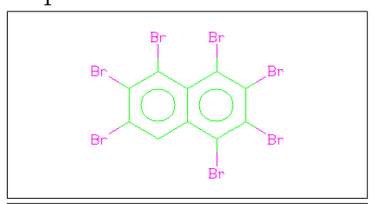
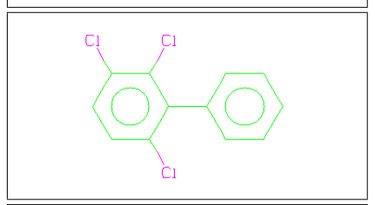
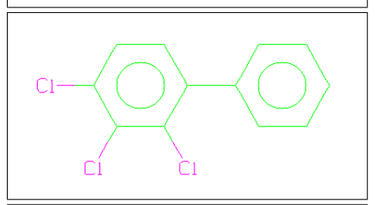
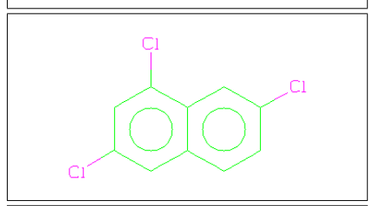
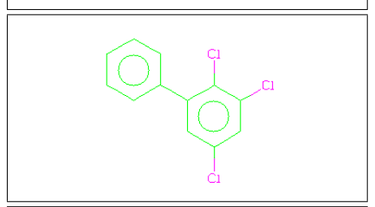
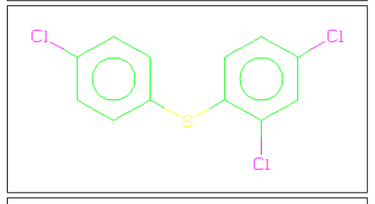
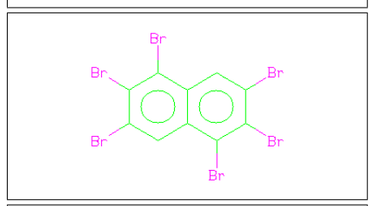
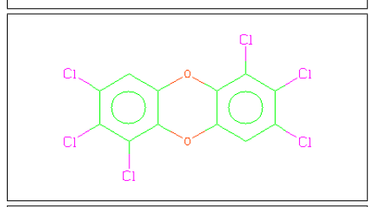
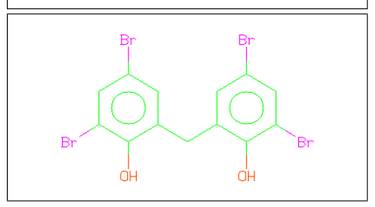
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
334	38998-75-3	`Clc1cc2c(oc3c(Cl)c(Cl)c(Cl)c(Cl)c23)c(Cl)c1Cl`		$5.28e+02$	$3.63e+03$	$1.23e+04$	$1.68e-07$	$1.23e-05$	$4.54e+02$	8.075	*No*
335	39001-02-0	`Clc1c(Cl)c2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl`		$8.63e+02$	$1.30e+03$	$2.41e+04$	$2.58e-08$	$2.28e-06$	$1.00e+03$	8.735	*No*
336	39073-07-9	`Brc1ccc2Oc3cc(Br)ccc3Oc2c1`		$6.49e+01$	$5.08e+03$	$2.11e+03$	$8.37e-05$	$3.00e-03$	$2.92e+00$	6.12	*No*
337	39239-77-5	`OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.21e+04$	$2.67e+03$	$5.05e+06$	$1.50e-07$	$1.17e-05$	$2.56e+00$	8.42	*Yes*
338	39485-83-1	`Clc1ccc(c(Cl)c1)c1c(Cl)cc(Cl)cc1Cl`		$1.87e+02$	$7.21e+04$	$6.76e+06$	$5.91e-06$	$2.99e-04$	$1.89e+01$	6.98	*No*
339	39568-98-4	`ClCc1c(Br)c(Br)c(CCl)c(Br)c1Br`		$2.75e+02$	$1.12e+04$	$3.82e+03$	$2.72e-06$	$1.60e-02$	$1.42e+01$	7.16	*Yes*
340	39568-99-5	`BrCc1c(Br)c(Br)c(CBr)c(Br)c1Br`		$1.91e+02$	$9.12e+03$	$4.69e+02$	$2.14e-06$	$1.40e-02$	$1.89e+01$	7.33	*Yes*
341	39569-21-6	`Clc1c(C)c(Br)c(Br)c(Br)c1Br`		$2.04e+02$	$1.12e+04$	$3.99e+04$	$1.63e-05$	$7.70e-04$	$5.61e+01$	6.74	*Yes*
342	40088-45-7	`Brc1cc(ccc1Br)c1cccc(Br)c1Br`		$1.39e+02$	$3.59e+04$	$4.63e+06$	$3.05e-06$	$1.71e-04$	$1.67e+01$	7.32	*No*

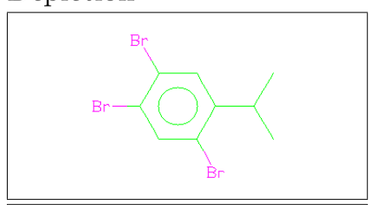
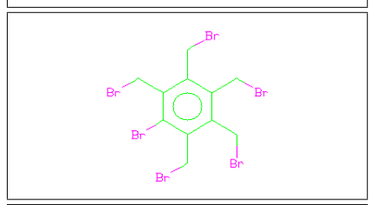
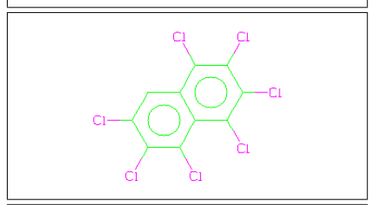
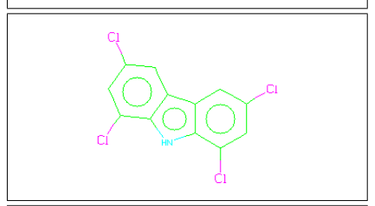
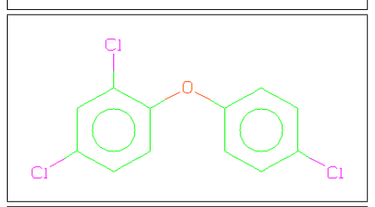
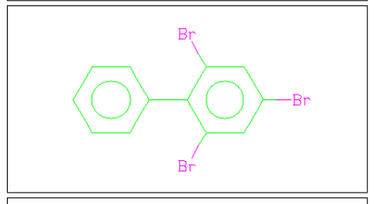
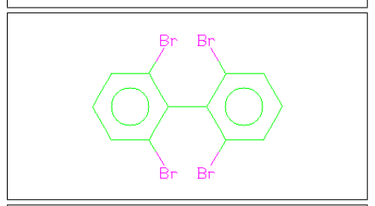
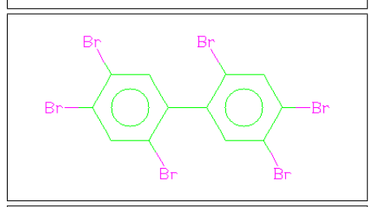
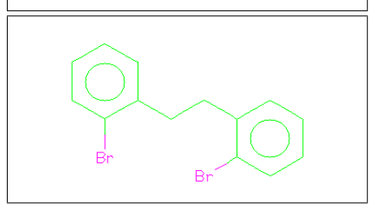
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
343	40356-57-8	`Clc1ccc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1Cl`		$9.62e+02$	$5.16e+03$	$5.54e+06$	$1.20e-07$	$9.15e-06$	$7.18e+01$	8.105	*No*
344	40723-69-1	`CCC(F)(F)C(F)(F)CCC(F)(F)C(F)(F)CC`		$1.17e+02$	$1.12e+04$	$6.00e+05$	$3.06e-06$	$1.63e-04$	$2.61e+01$	7.15	*No*
345	42115-16-2	`BrCC(Br)COc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$3.21e+02$	$1.64e+04$	$2.54e+06$	$1.63e-03$	$2.60e-02$	$2.76e+00$	6.89	*Yes*
346	42255-14-1	`Clc1c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1O`		$1.52e+03$	$2.37e+03$	$4.69e+05$	$9.36e-05$	$1.71e-05$	$1.72e+01$	8.53	*No*
347	43007-16-5	`Clc1ccc(cc1)C(=O)c1ccc(cc1)c1ccc(Br)cc1`		$6.99e+01$	$2.16e+03$	$2.72e+05$	$3.40e-05$	$1.47e-03$	$2.38e+00$	6.45	*Yes*
348	47726-62-5	`Clc1cc(Cl)c(O)c(c1)c1nc2c(Cl)c3oc(nc3c(Cl)c2o1)c1cc(Cl)cc(Cl)c1O`		$5.22e+02$	$4.94e+03$	$5.08e+03$	$3.75e-04$	$5.00e-03$	$3.36e+00$	7.88	*Yes*
349	49693-20-1	`Brc1cc(Br)c(NC(=O)c2ccccc(c2)C(=O)Nc2c(Br)cc(Br)cc2Br)c(Br)c1`		$9.19e+02$	$9.02e+03$	$1.64e+03$	$9.88e-04$	$2.80e-02$	$5.02e+00$	6.5	*No*
350	50274-96-9	`Clc1ccc(Cc2ccc(cc2Cl)N(=O)=O)c(Cl)c1`		$1.35e+02$	$2.96e+03$	$1.76e+04$	$2.27e-04$	$8.00e-03$	$4.68e+00$	5.77	*Yes*
351	50285-18-2	`FC(F)(C(F)(F)F)C(F)(C(F)(C(F)(F)F)C(F)(F)F)C(F)(C(F)(F)F)C(F)(F)F`		$2.18e+04$	$1.43e+04$	$7.28e+06$	$1.51e-05$	$7.23e-04$	$1.00e+06$	6.8	*Yes*

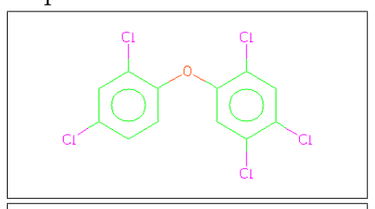
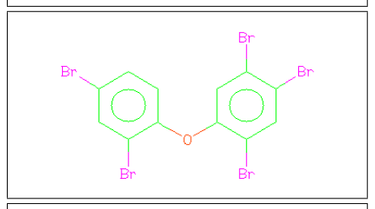
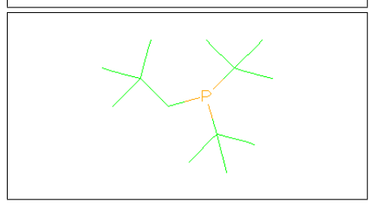
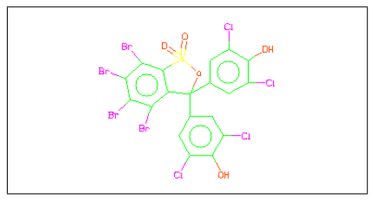
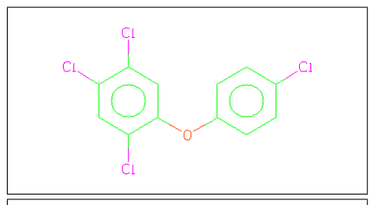
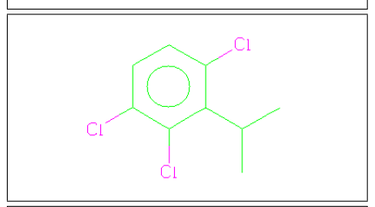
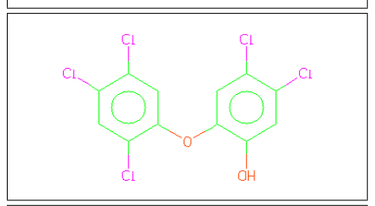
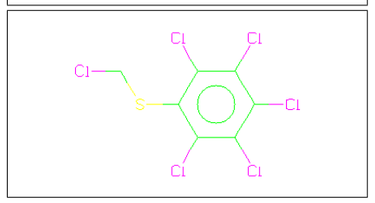
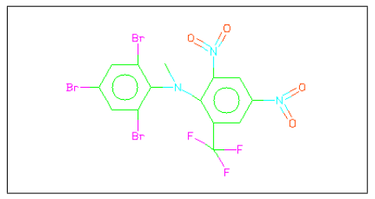
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
352	50585-37-0	`Brc1cc2Oc3ccccc3Oc2cc1Br`		$6.49e+01$	$5.08e+03$	$2.11e+03$	$8.37e-05$	$3.00e-03$	$3.93e+00$	6.12	*No*
353	50585-40-5	`Clc1cc2Oc3cc(Br)c(Br)cc3Oc2cc1Cl`		$1.73e+02$	$8.37e+03$	$3.79e+04$	$2.01e-06$	$1.15e-04$	$1.51e+01$	7.41	*No*
354	50585-41-6	`Brc1cc2Oc3cc(Br)c(Br)cc3Oc2cc1Br`		$1.91e+02$	$4.81e+03$	$1.87e+04$	$5.50e-07$	$3.66e-05$	$1.62e+01$	7.9	*No*
355	50585-43-8	`Fc1cc2Oc3cc(Br)c(Br)cc3Oc2cc1F`		$3.06e+02$	$9.34e+03$	$3.36e+03$	$2.74e-05$	$1.21e-03$	$9.67e+00$	6.52	*No*
356	50594-82-6	`Clc1cc(cc(Cl)c1Cl)C(F)(F)F`		$1.66e+02$	$7.82e+02$	$5.36e+03$	$3.00e-03$	$7.00e-02$	$2.51e+02$	4.89	*Yes*
357	51735-74-1	`O=S(OS(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$3.99e+03$	$4.70e+03$	$4.50e+06$	$5.70e-07$	$3.81e-05$	$1.00e+06$	7.92	*No*
358	51775-36-1	`ClC[C@@]12[C@@H](Cl)[C@@H](Cl)[C@@H](CC1(Cl)Cl)C2(CCl)CCl`		$9.47e+02$	$1.31e+03$	$3.45e+04$	$2.08e-05$	$9.44e-04$	$4.56e+00$	5.92	*No*
359	52117-16-5	`Brc1ccc(cc1)N=C(Cl)c1cc(Cl)cc(Br)c1O`		$1.27e+02$	$2.80e+03$	$1.94e+04$	$1.00e-02$	$4.00e-03$	$3.83e+00$	6.07	*Yes*
360	52135-26-9	`Clc1c(Cl)c2C(=NC(Cl)(Cl)c2c(Cl)c1Cl)Cl`		$5.27e+02$	$8.05e+03$	$4.95e+06$	$1.03e-06$	$7.00e-03$	$4.92e+01$	7.45	*No*

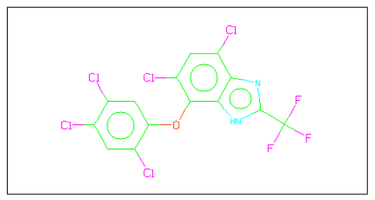
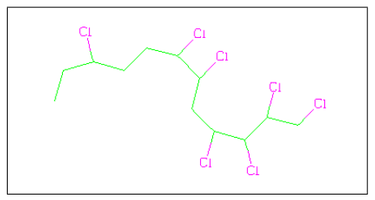
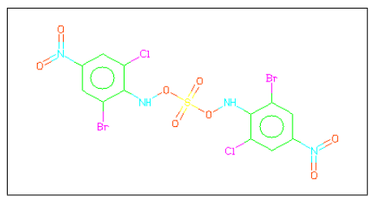
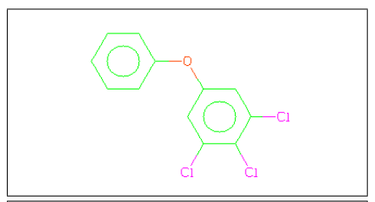
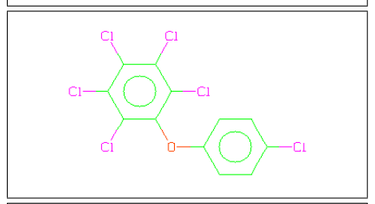
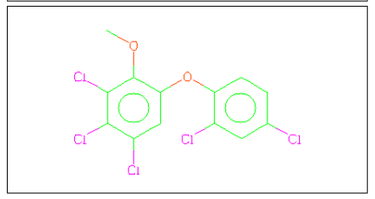
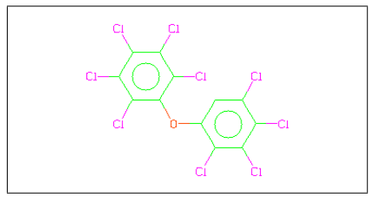
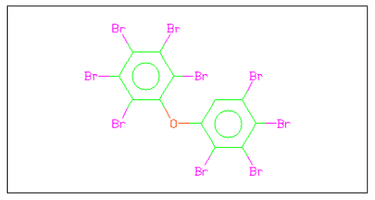
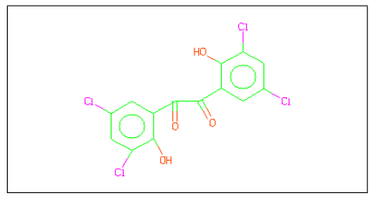
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
361	52176-20-2	`Brc1cc(Br)c(OCOc2c(Br)cc(Br)cc2Br)c(Br)c1`		$5.97e+02$	$1.16e+03$	$2.30e+06$	$1.63e-08$	$1.57e-06$	$2.51e+00$	9.16	*Yes*
362	52184-14-2	`O=N(=O)c1ccccc1N=Nc1cc(cc(c1O)C(C)(C)C)C(C)(C)C`		$1.49e+02$	$6.00e+00$	$4.16e+04$	$1.66e-05$	$1.18e-05$	$5.06e+00$	8.55	*Yes*
363	52184-19-7	`CCC(C)(C)c1cc(N=Nc2cccc2N(=O)=O)c(O)c(c1)C(C)(C)CC`		$1.66e+02$	$6.00e+00$	$2.01e+04$	$1.79e-05$	$1.34e-06$	$2.42e+00$	9.53	*Yes*
364	52184-29-9	`Clc1ccc(N=Nc2cc(cc(c2O)C(C)(C)C)C(C)(C)C)c(c1)N(=O)=O`		$2.44e+02$	$6.00e+00$	$3.27e+04$	$1.82e-05$	$2.95e-06$	$5.10e+00$	9.19	*Yes*
365	52663-77-1	`Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)c1c(Cl)c(Cl)cc(Cl)c1Cl`		$1.34e+03$	$1.38e+04$	$6.10e+06$	$3.35e-09$	$3.64e-07$	$3.25e+02$	8.86	*No*
366	52819-39-3	`ClCC1(CCl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2(Cl)Cl`		$2.25e+03$	$1.86e+04$	$5.95e+06$	$8.21e-06$	$4.15e-04$	$5.72e+00$	6.98	*No*
367	53097-60-2	`BrCCc1c(Br)c(Br)c(Br)c(Br)c1Br`		$2.90e+02$	$5.25e+03$	$3.92e+04$	$8.05e-07$	$5.23e-05$	$1.34e+01$	7.82	*Yes*
368	53555-65-0	`Clc1cc(Cl)c2cc(Cl)c(Cl)c(Cl)c2c1`		$1.70e+02$	$2.95e+04$	$4.81e+05$	$3.24e-05$	$1.38e-03$	$2.59e+01$	6.39	*No*
369	53555-66-1	`Clc1c(Cl)cc(cc1Cl)c1ccccc1`		$6.75e+01$	$1.02e+04$	$5.61e+04$	$2.33e-04$	$8.00e-03$	$6.94e+00$	5.69	*No*

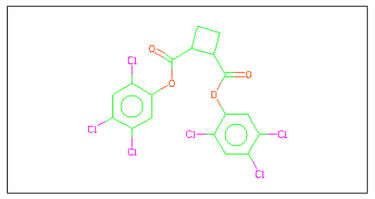
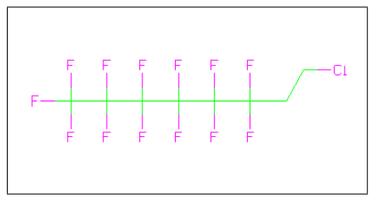
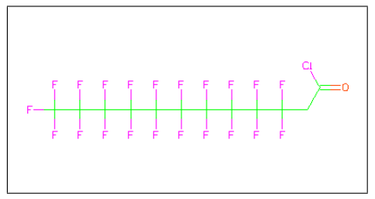
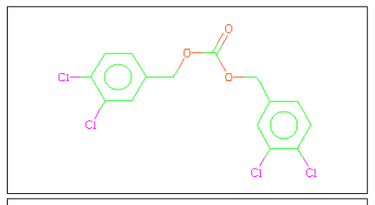
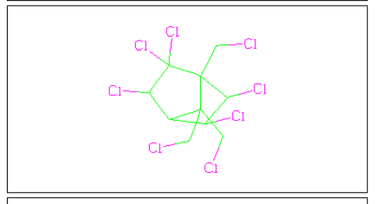
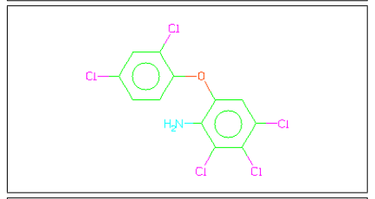
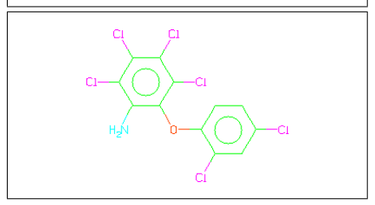
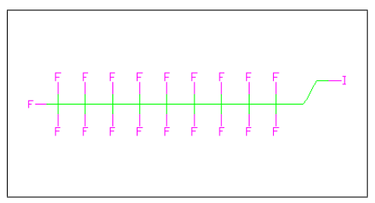
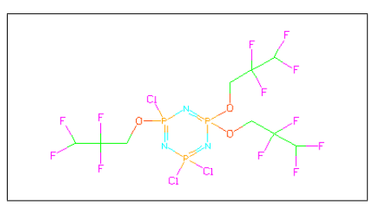
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
370	53643-52-0	`Brc1ccc(cc1)OC(=O)c1cc(Br)cc(Br)c1O`		$7.25e+01$	$8.90e+03$	$2.94e+02$	$1.40e-04$	$1.67e-03$	$8.45e+00$	6.49	*No*
371	54230-22-7	`Clc1c(Cl)cc(Cl)c(c2cccc2)c1Cl`		$1.10e+02$	$2.71e+04$	$4.66e+05$	$3.74e-05$	$1.56e-03$	$1.33e+01$	6.34	*No*
372	54965-70-7	`Clc1cc(Cl)c(C(C)C)c(Cl)c1`		$7.01e+01$	$1.65e+03$	$5.75e+03$	$5.16e-04$	$1.60e-02$	$3.46e+00$	5.38	*No*
373	55044-46-7	`ClC(=C1C(Cl)C(Cl)C1=C(Cl)Cl)Cl`		$1.63e+02$	$1.04e+03$	$1.69e+04$	$1.52e-03$	$7.30e-02$	$1.97e+01$	5.08	*No*
374	55191-16-7	`COc1c(Cl)cc(cc1Cl)C(C)(C)C`		$7.14e+01$	$1.40e+03$	$6.11e+04$	$7.51e-04$	$2.30e-02$	$3.37e+00$	5.27	*No*
375	55521-14-7	`COC(=O)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(=O)OC`		$1.40e+03$	$5.64e+03$	$1.88e+05$	$5.55e-04$	$4.80e-02$	$2.46e+01$	6.19	*No*
376	55570-84-8	`ClC12C3C4(Cl)C(Cl)(C2(Cl)Cl)C2(Cl)C1C3(Cl)C(Cl)(Cl)C42Cl`		$2.14e+04$	$1.71e+04$	$3.77e+06$	$2.92e-05$	$1.31e-03$	$1.40e+01$	6.92	*No*
377	55591-23-6	`FC(F)(C(F)(F)C(F)(F)S(=O)(=O)Cl)C(F)(F)C(F)(F)C(F)(F)F`		$6.83e+02$	$1.45e+04$	$2.77e+05$	*NA*	$6.48e-03$	$1.00e+06$	6.81	*Yes*
378	55682-71-8	`FC(F)(F)c1ccc(cc1)c1nc(nc(n1)c1ccc(cc1)C(F)(F)F)c1ccc(cc1)C(F)(F)F`		$1.42e+03$	$1.34e+03$	$9.18e+06$	$2.86e-04$	$1.16e-05$	$5.10e+00$	7.98	*No*

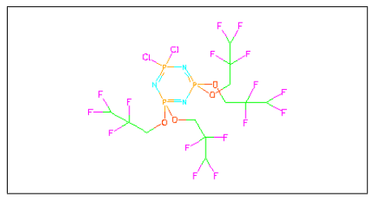
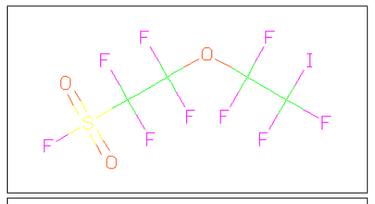
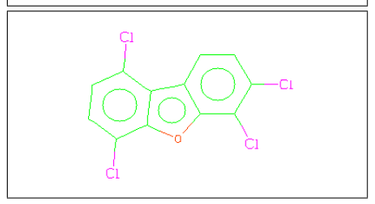
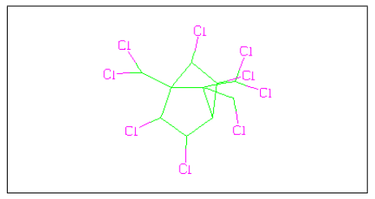
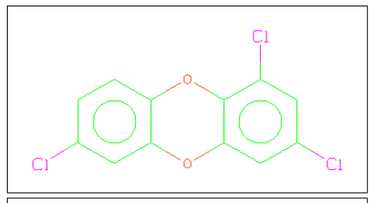
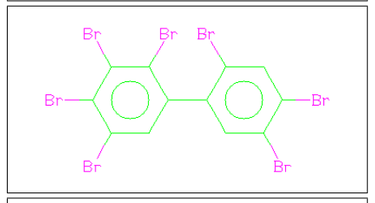
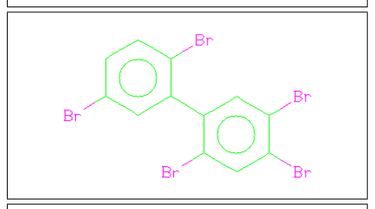
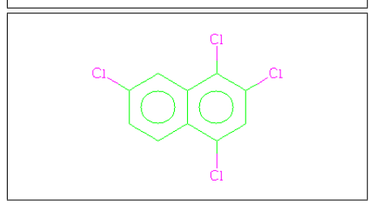
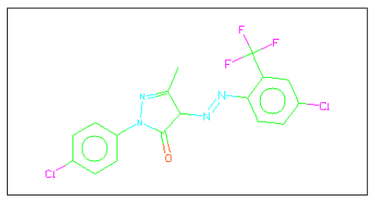
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
379	55688-01-2	`Brc1cc2c(c(Br)c1Br)c(Br)c(Br)c(Br)c2Br`		$6.34e+02$	$3.42e+03$	$1.12e+05$	$7.95e-09$	$8.24e-07$	$1.98e+02$	9.4	*No*
380	55702-45-9	`Clc1ccc(Cl)c(Cl)c1c1ccccc1`		$6.75e+01$	$9.86e+03$	$5.23e+04$	$2.33e-04$	$8.00e-03$	$8.52e+00$	5.68	*No*
381	55702-46-0	`Clc1ccc(c2ccccc2)c(Cl)c1Cl`		$6.75e+01$	$1.32e+04$	$9.90e+04$	$2.33e-04$	$8.00e-03$	$8.52e+00$	5.775	*No*
382	55720-37-1	`Clc1cc(Cl)c2cc(Cl)ccc2c1`		$6.35e+01$	$1.28e+04$	$1.47e+04$	$1.25e-03$	$3.60e-02$	$5.32e+00$	5.225	*No*
383	55720-44-0	`Clc1cc(Cl)c(Cl)c(c1)c1ccccc1`		$6.75e+01$	$1.02e+04$	$5.61e+04$	$2.33e-04$	$8.00e-03$	$6.94e+00$	5.69	*No*
384	55759-88-1	`Clc1ccc(cc1)Sc1ccc(Cl)cc1Cl`		$7.94e+01$	$5.94e+03$	$6.33e+05$	$5.19e-05$	$2.00e-03$	$2.26e+00$	6.22	*No*
385	56480-06-9	`Brc1c(Br)cc2c(Br)c(Br)c(Br)cc2c1Br`		$3.70e+02$	$9.34e+03$	$3.38e+05$	$1.05e-07$	$8.34e-06$	$8.43e+01$	8.51	*Yes*
386	57653-85-7	`Clc1cc2Oc3c(cc(Cl)c(Cl)c3Cl)Oc2c(Cl)c1Cl`		$4.21e+02$	$5.36e+03$	$4.79e+04$	$1.69e-07$	$1.23e-05$	$3.41e+01$	8.21	*No*
387	57863-93-1	`Brc1cc(Cc2cc(Br)cc(Br)c2O)c(O)c(Br)c1`		$1.55e+02$	$1.08e+04$	$1.83e+02$	$4.00e-03$	$4.90e-02$	$2.77e+00$	6.62	*Yes*

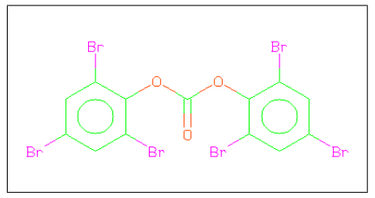
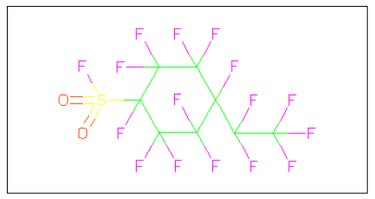
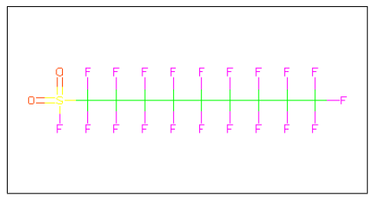
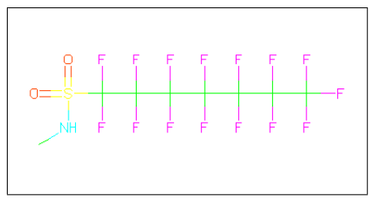
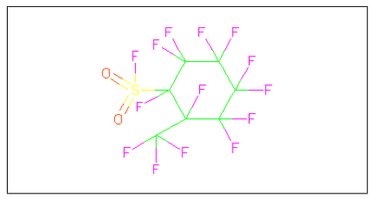
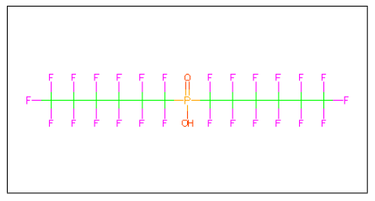
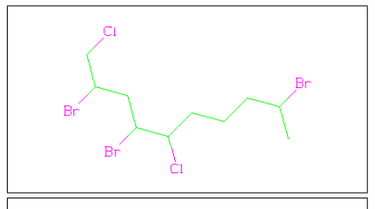
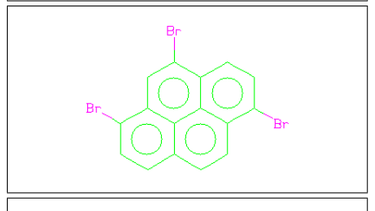
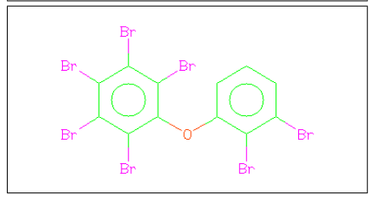
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
388	58683-70-8	`CC(C)c1cc(Br)c(Br)cc1Br`		$8.10e+01$	$5.06e+03$	$1.17e+04$	$8.80e-05$	$3.00e-03$	$4.21e+00$	6.12	*Yes*
389	58828-53-8	`BrCc1c(CBr)c(CBr)c(Br)c(CBr)c1CBr`		$9.53e+01$	$9.10e+03$	$5.42e+00$	$2.28e-06$	$1.50e-02$	$6.42e+00$	7.34	*Yes*
390	58863-14-2	`Clc1cc2c(c(Cl)c1Cl)c(Cl)c(Cl)c(Cl)c2Cl`		$4.53e+02$	$1.32e+04$	$2.85e+06$	$7.95e-07$	$4.95e-05$	$1.26e+02$	7.94	*No*
391	58910-96-6	`Clc1cc(Cl)c2[nH]c3c(Cl)cc(Cl)cc3c2c1`		$1.21e+02$	$2.89e+03$	$5.59e+03$	$1.93e-04$	$7.00e-03$	$6.34e+00$	5.78	*No*
392	59039-21-3	`Clc1ccc(cc1)Oc1ccc(Cl)cc1Cl`		$8.25e+01$	$3.57e+03$	$1.16e+05$	$1.30e-03$	$3.80e-02$	$6.51e+00$	5.335	*No*
393	59080-33-0	`Brc1cc(Br)c(c(Br)c1)c1ccccc1`		$7.80e+01$	$1.13e+04$	$5.17e+04$	$3.78e-05$	$1.63e-03$	$7.64e+00$	6.23	*No*
394	59080-37-4	`Brc1cccc(Br)c1c1c(Br)cccc1Br`		$1.39e+02$	$5.72e+04$	$5.28e+06$	$3.05e-06$	$1.71e-04$	$1.64e+01$	6.91	*No*
395	59080-40-9	`Brc1cc(Br)c(Br)cc1c1cc(Br)c(Br)cc1Br`		$4.08e+02$	$4.81e+03$	$1.13e+06$	$1.83e-08$	$1.74e-06$	$8.30e+01$	9.1	*No*
396	59485-34-6	`Brc1ccccc1CCc1ccccc1Br`		$6.83e+01$	$9.30e+03$	$1.71e+05$	$2.49e-05$	$1.10e-03$	$2.02e+00$	6.52	*Yes*

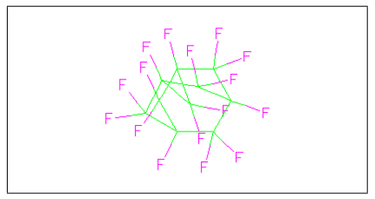
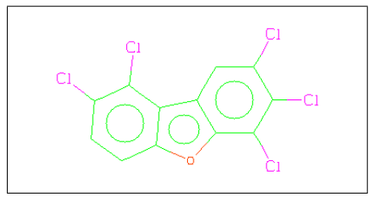
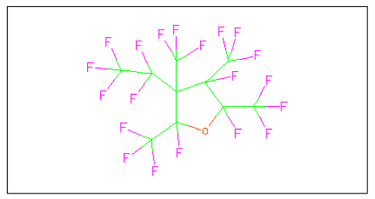
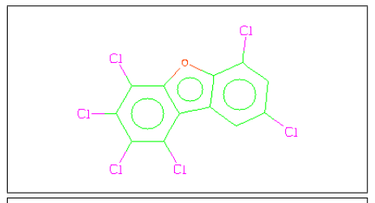
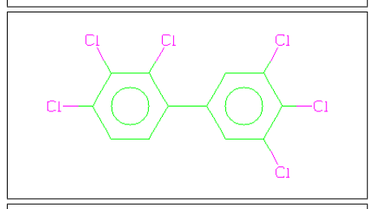
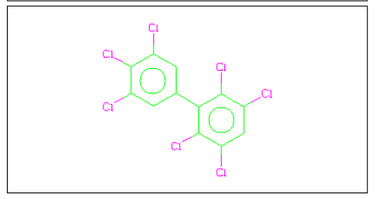
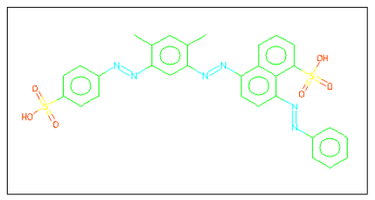
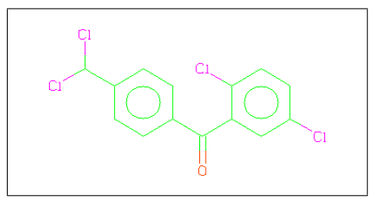
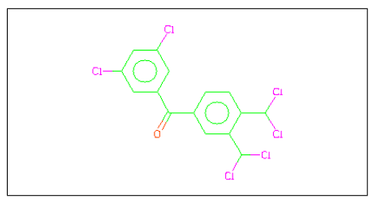
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
397	60123-64-0	`Clc1ccc(Oc2cc(Cl)c(Cl)cc2Cl)c(Cl)c1`		$2.20e+02$	$1.10e+04$	$1.63e+06$	$3.26e-05$	$1.40e-03$	$1.56e+01$	6.405	*No*
398	60348-60-9	`Brc1ccc(Oc2cc(Br)c(Br)cc2Br)c(Br)c1`		$2.80e+02$	$1.51e+04$	$2.36e+06$	$1.30e-06$	$8.02e-05$	$1.94e+01$	7.25	*No*
399	60633-21-8	`CC(C)(C)CP(C(C)(C)C)C(C)(C)C`		$6.17e+01$	$3.91e+03$	$1.87e+04$	$8.95e-05$	$3.00e-03$	$4.03e+00$	5.95	*No*
400	61053-97-2	`Clc1cc(cc(Cl)c1O)C1(OS(=O)(=O)c2c(Br)c(Br)c(Br)c(Br)c12)c1cc(Cl)c(O)c(Cl)c1`		$2.54e+03$	$9.44e+02$	$1.24e+04$	*NA*	$3.69e-05$	$3.30e+00$	9.34	*Yes*
401	61328-45-8	`Clc1ccc(cc1)Oc1cc(Cl)c(Cl)cc1Cl`		$1.35e+02$	$7.32e+03$	$6.26e+05$	$2.08e-04$	$7.00e-03$	$1.14e+01$	5.89	*No*
402	61465-79-0	`Clc1ccc(Cl)c(C(C)C)c1Cl`		$7.01e+01$	$1.65e+03$	$5.75e+03$	$5.16e-04$	$1.60e-02$	$4.09e+00$	5.38	*No*
403	61639-90-5	`Oc1cc(Cl)c(Cl)cc1Oc1cc(Cl)c(Cl)cc1Cl`		$2.13e+02$	$3.93e+03$	$9.46e+03$	$1.00e-02$	$5.00e-03$	$2.74e+00$	5.95	*No*
404	62601-17-6	`ClCSc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.58e+02$	$4.70e+03$	$7.95e+04$	$9.46e-05$	$4.00e-03$	$3.66e+00$	6.07	*Yes*
405	63333-35-7	`Brc1cc(Br)c(c(Br)c1)N(C)c1c(cc(cc1C(F)(F)F)N(=O)=O)N(=O)=O`		$1.14e+03$	$6.14e+03$	$8.82e+03$	$1.40e-02$	$7.00e-03$	$5.18e+00$	7.68	*Yes*

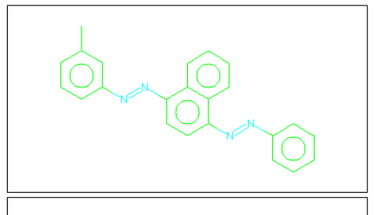
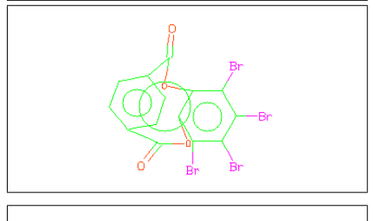
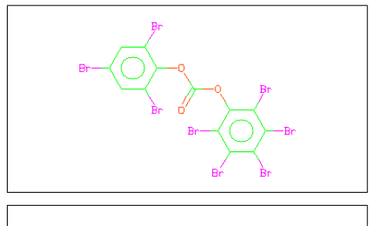
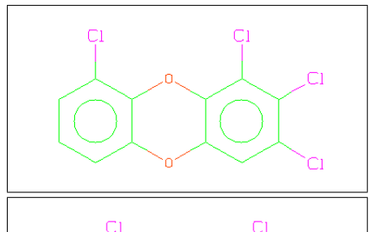
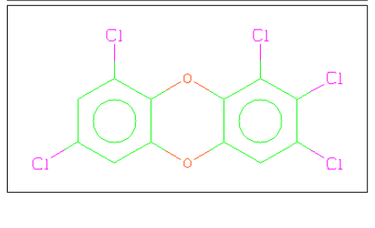
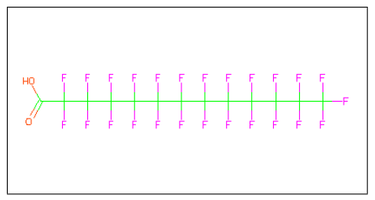
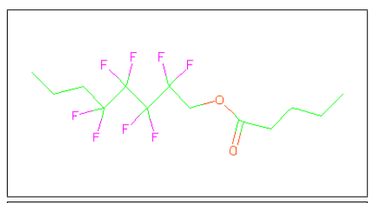
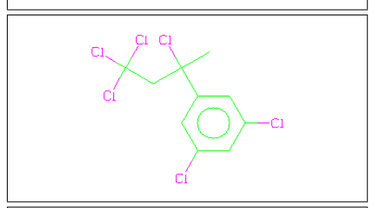
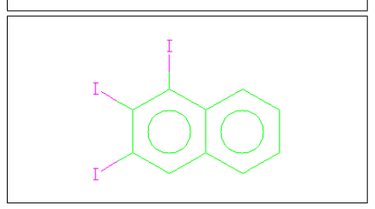
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
406	63405-99-2	`Clc1cc(Cl)c(Cl)cc1Oc1c(Cl)cc(Cl)c2nc([nH]c12)C(F)(F)F`		$8.14e+02$	$1.11e+04$	$6.04e+05$	NA	$1.03e-02$	$9.34e+00$	6.64	Yes
407	63449-39-8	`CCC(Cl)CCC(Cl)C(Cl)CC(Cl)C(Cl)C(Cl)CCl`		$3.54e+02$	$6.98e+03$	$4.24e+05$	$1.23e-06$	$7.44e-05$	$2.77e+00$	6	Yes
408	63589-34-4	`Clc1cc(cc(Br)c1NOS(=O)(=O)ONc1c(Cl)cc(cc1Br)N(=O)=O)N(=O)=O`		$5.22e+02$	$1.14e+04$	$1.52e+04$	$1.77e-03$	$2.10e-02$	$4.33e+01$	7.13	No
409	63646-53-7	`Clc1c(Cl)cc(Oc2ccccc2)cc1Cl`		$7.94e+01$	$2.68e+03$	$8.58e+03$	$1.02e-04$	$4.00e-03$	$3.84e+00$	5.84	No
410	63646-56-0	`Clc1ccc(cc1)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$3.60e+02$	$1.79e+04$	$3.19e+06$	$5.08e-06$	$2.64e-04$	$1.71e+01$	7.015	No
411	63709-64-8	`COc1c(Oc2ccc(Cl)cc2Cl)cc(Cl)c(Cl)c1Cl`		$2.74e+02$	$9.21e+03$	$4.35e+06$	$2.78e-05$	$1.22e-03$	$6.34e+00$	6.51	No
412	63919-04-0	`Clc1cc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl`		$1.57e+03$	$3.98e+03$	$5.25e+06$	$1.83e-08$	$1.69e-06$	$1.21e+02$	8.54	No
413	63936-56-1	`Brc1cc(Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c(Br)c1Br`		$2.42e+03$	$1.14e+02$	$9.40e+03$	$4.09e-11$	$7.27e-09$	$1.61e+02$	11.22	Yes
414	63992-65-4	`Clc1cc(Cl)c(O)c(c1)C(=O)C(=O)c1cc(Cl)cc(Cl)c1O`		$1.32e+02$	$1.28e+04$	$8.82e+02$	$2.00e-03$	$2.90e-02$	$1.27e+01$	6.73	No

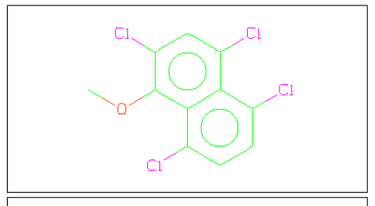
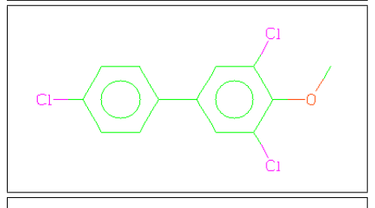
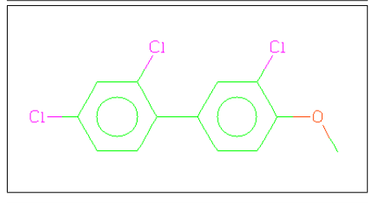
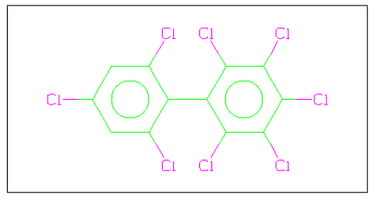
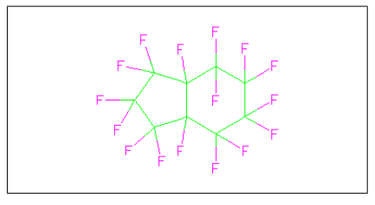
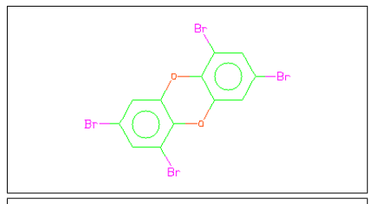
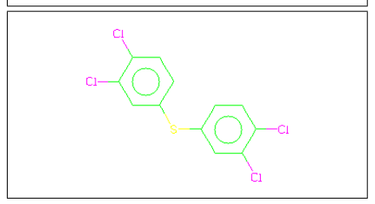
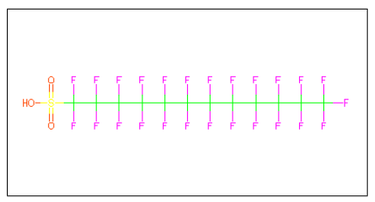
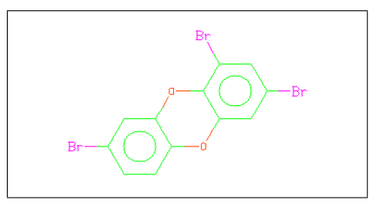
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
415	64011-98-9	O=C(Oc1cc(Cl)c(Cl)cc1Cl)C1CCC1C(=O)Oc1cc(Cl)c(Cl)cc1Cl		$3.25e+02$	$8.21e+03$	$3.83e+03$	$3.88e-06$	$4.00e-03$	$6.24e+00$	7.43	*No*
416	64018-25-3	ClCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$8.03e+02$	$5.12e+03$	$3.83e+05$	*NA*	$2.84e-02$	$2.42e+01$	6.13	*Yes*
417	64018-26-4	ClC(=O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$5.91e+03$	$1.33e+04$	$2.19e+06$	*NA*	$1.06e-02$	$9.47e+03$	6.75	*Yes*
418	64057-76-7	O=C(OCc1ccc(Cl)c(Cl)c1)OCc1ccc(Cl)c(Cl)c1		$1.61e+02$	$5.97e+03$	$1.80e+04$	$3.32e-04$	$3.10e-02$	$2.15e+00$	6.23	*No*
419	64618-67-3	ClCC12C(Cl)C(Cl)C(C(Cl)C2(Cl)Cl)C1(CCl)CCl		$1.46e+03$	$2.85e+03$	$3.47e+05$	$1.31e-05$	$6.28e-04$	$5.35e+00$	6.265	*No*
420	64630-64-4	Clc1ccc(Oc2cc(Cl)c(Cl)c(Cl)c2N)c(Cl)c1		$2.95e+02$	$2.02e+03$	$6.67e+03$	$4.74e-04$	$2.58e-01$	$9.12e+00$	5.52	*No*
421	64630-65-5	Clc1ccc(Oc2c(N)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1		$4.82e+02$	$5.38e+03$	$5.08e+04$	$1.80e-04$	$8.70e-02$	$3.19e+00$	6.16	*No*
422	65510-56-7	ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$4.54e+03$	$2.10e+03$	$1.41e+06$	$7.33e-08$	$6.07e-06$	$1.73e+01$	8.64	*Yes*
423	65601-41-4	FC(F)C(F)(F)COP1(=NP(=NP(=N1)(OCC(F)(F)C(F)F)OCC(F)(F)C(F)F)(Cl)Cl)Cl		$3.07e+02$	$1.03e+04$	$8.41e+03$	$3.77e-05$	$1.70e-03$	$1.03e+01$	6.59	*No*

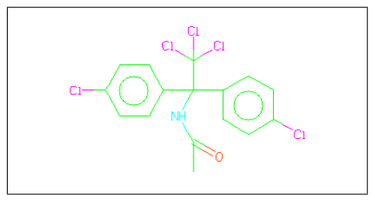
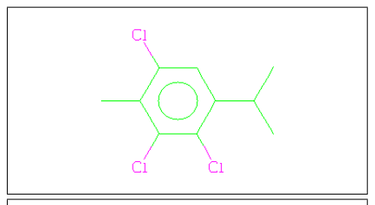
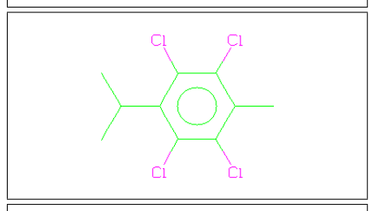
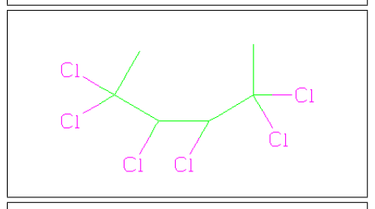
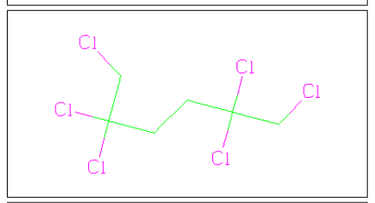
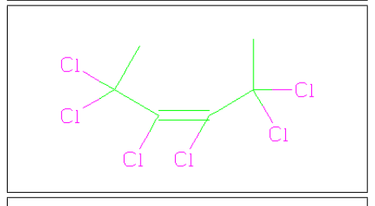
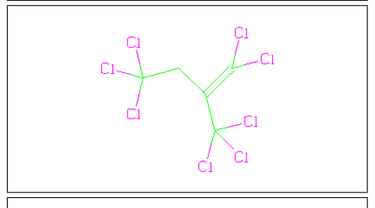
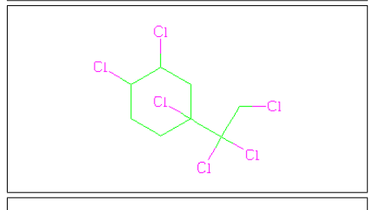
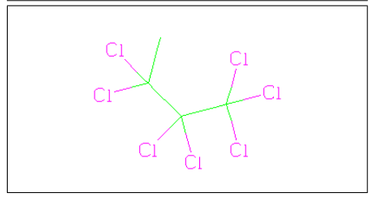
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
424	65601-42-5	FC(F)C(F)(F)COP1(=NP(=NP(=N1)(Cl)Cl)(OCC(F)(F)C(F)F)OCC(F)(F)C(F)F)OCC(F)(F)C(F)F		$6.41e+02$	$6.58e+03$	$4.21e+05$	$1.87e-06$	$1.14e-04$	$7.75e+00$	7.62	*No*
425	66137-74-4	FC(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)I		$2.02e+02$	$7.92e+03$	$3.05e+03$	*NA*	$1.66e-02$	$1.00e+06$	6.41	*Yes*
426	66794-59-0	Clc1ccc2c(oc3c(Cl)ccc(Cl)c23)c1Cl		$1.21e+02$	$6.59e+03$	$3.94e+03$	$4.45e-05$	$1.84e-03$	$4.23e+01$	6.29	*No*
427	66860-80-8	ClCC1(C(Cl)Cl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2Cl		$1.56e+03$	$3.80e+03$	$8.62e+05$	$7.78e-05$	$3.00e-03$	$5.12e+00$	6.08	*No*
428	67028-17-5	Clc1ccc2Oc3c(cc(Cl)cc3Cl)Oc2c1		$9.64e+01$	$6.42e+03$	$8.26e+03$	$4.41e-05$	$1.81e-03$	$3.92e+00$	6.28	*No*
429	67733-52-2	Brc1cc(Br)c(Br)cc1c1cc(Br)c(Br)c(Br)c1Br		$7.00e+02$	$1.76e+03$	$2.15e+05$	$1.38e-09$	$1.71e-07$	$1.31e+02$	9.99	*No*
430	67888-96-4	Brc1ccc(Br)c(c1)c1cc(Br)c(Br)cc1Br		$2.38e+02$	$4.58e+04$	$3.25e+06$	$2.39e-07$	$1.74e-05$	$3.78e+01$	7.655	*No*
431	67922-21-8	Clc1ccc2c(Cl)cc(Cl)c(Cl)c2c1		$1.04e+02$	$1.11e+04$	$5.95e+04$	$2.03e-04$	$7.00e-03$	$1.17e+01$	5.75	*No*
432	67923-41-5	Clc1ccc(cc1)N1N=C(C)C(N=Nc2ccc(Cl)cc2C(F)(F)F)C1=O		$3.69e+02$	$1.00e+01$	$3.64e+06$	$1.94e-05$	$7.78e-05$	$2.13e+00$	6.8	*Yes*

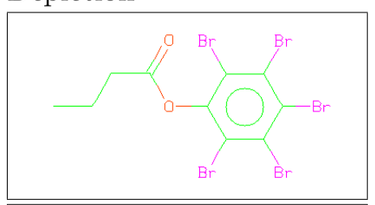
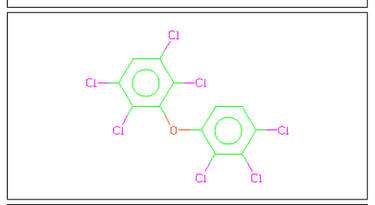
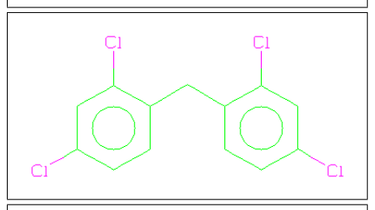
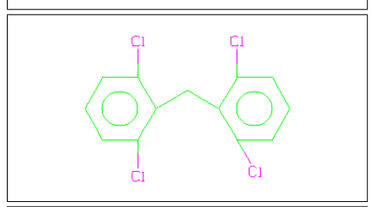
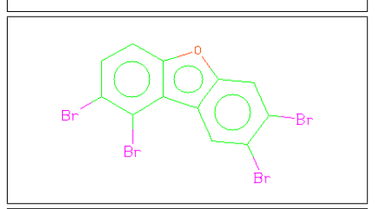
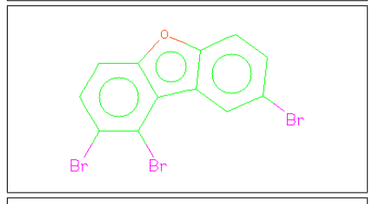
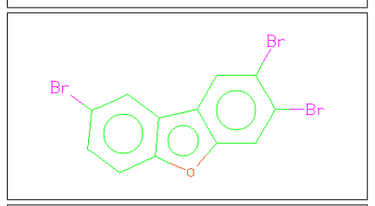
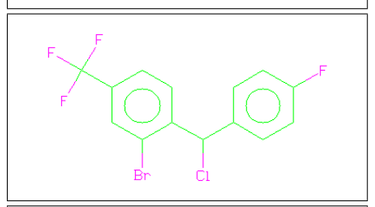
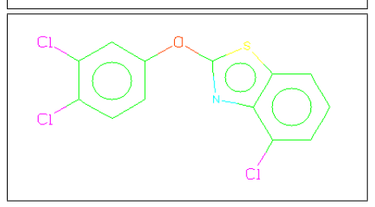
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
433	67990-32-3	O=C(Oc1c(Br)cc(Br)cc1Br)Oc1c(Br)cc(Br)cc1Br		$5.14e+02$	$2.32e+03$	$6.53e+05$	$6.48e-08$	$7.77e-04$	$1.50e+01$	8.55	*Yes*
434	68156-06-9	FC1(S(=O)(=O)F)C(F)(F)C(F)(F)C(F)(C(F)(F)C1(F)F)C(F)(F)C(F)(F)F		$1.70e+03$	$5.65e+03$	$1.35e+06$	$3.53e-04$	$5.00e-03$	$1.00e+06$	7.76	*Yes*
435	68259-06-3	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)F		$3.44e+03$	$2.44e+03$	$3.66e+06$	$1.43e-04$	$1.33e-03$	$1.00e+06$	8.5	*Yes*
436	68259-14-3	CNS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.17e+03$	$2.30e+03$	$4.35e+04$	$2.00e-03$	$8.50e-02$	$8.46e+00$	5.6	*Yes*
437	68318-34-3	FC1(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C1(F)S(=O)(=O)F		$9.70e+02$	$2.81e+03$	$1.18e+04$	$6.00e-03$	$2.01e-01$	$1.00e+06$	5.73	*Yes*
438	68412-69-1	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)P(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.12e+04$	$1.82e+04$	$7.82e+06$	$1.34e-05$	$6.76e-04$	$7.64e+01$	6.96	*Yes*
439	68512-16-3	ClCC(Br)CC(Br)C(Cl)CCCC(C)Br		$7.79e+01$	$8.99e+03$	$1.52e+03$	$3.51e-05$	$1.54e-03$	$2.46e+00$	6.5	*No*
440	68519-97-1	Brc1ccc2ccc3c(Br)ccc4c(Br)cc1c2c34		$3.91e+02$	$2.60e+04$	$6.56e+02$	*NA*	$1.10e-03$	$2.79e+00$	7.6	*Yes*
441	68928-80-3	Brc1cccc(Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c1Br		$8.24e+02$	$8.48e+02$	$2.17e+05$	$7.46e-09$	$7.83e-07$	$3.55e+01$	9.44	*Yes*

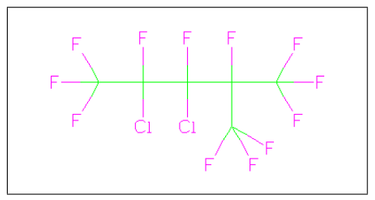
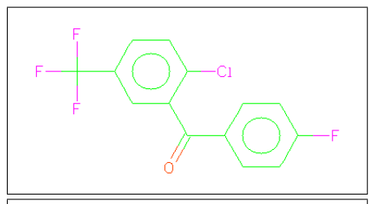
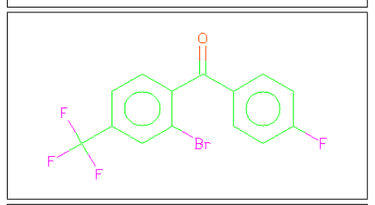
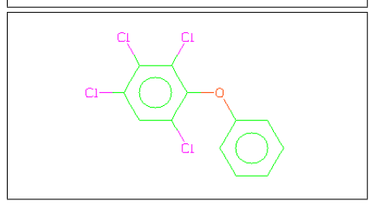
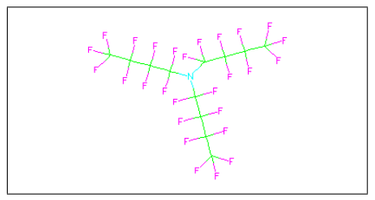
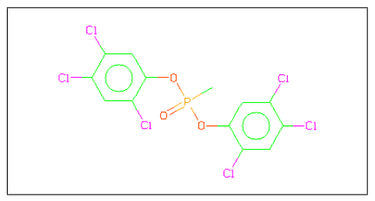
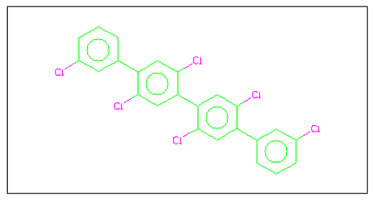
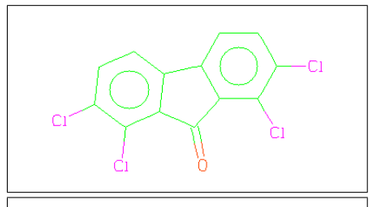
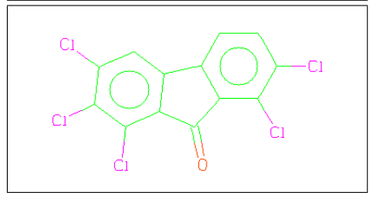
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
442	69064-33-1	FC12C(F)(F)C3(F)C(F)(F)C(F)(C1(F)F)C(F)(F)C(F)(C2(F)F)C3(F)F		$1.81e+03$	$7.75e+03$	$2.07e+05$	$4.46e-05$	$1.90e-03$	$1.00e+06$	6.4	*No*
443	69433-00-7	Clc1c(Cl)cc2c(oc3ccc(Cl)c(Cl)c23)c1Cl		$1.98e+02$	$5.64e+03$	$1.53e+04$	$7.00e-06$	$3.50e-04$	$9.33e+01$	6.705	*No*
444	69661-30-9	FC(F)(F)C1(C(F)(F)C(F)(F)F)C(F)(OC(F)(C(F)(F)F)C1(F)C(F)(F)F)C(F)(F)F		$3.56e+04$	$1.03e+04$	$7.15e+06$	*NA*	$3.11e-03$	$1.00e+06$	7.22	*Yes*
445	69698-60-8	Clc1cc(Cl)c2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c1		$3.23e+02$	$6.90e+03$	$6.47e+04$	$1.09e-06$	$6.59e-05$	$2.06e+02$	7.58	*No*
446	69782-90-7	Clc1ccc(c2cc(Cl)c(Cl)c(Cl)c2)c(Cl)c1Cl		$3.06e+02$	$2.61e+04$	$9.38e+06$	$9.23e-07$	$5.65e-05$	$4.57e+01$	7.61	*No*
447	69782-91-8	Clc1c(Cl)cc(cc1Cl)c1c(Cl)c(Cl)cc(Cl)c1Cl		$5.01e+02$	$1.23e+04$	$7.04e+06$	$1.43e-07$	$1.06e-05$	$7.64e+01$	8.27	*No*
448	70660-63-8	Cc1cc(C)c(N=Nc2ccc(cc2)S(=O)(=O)O)cc1N=Nc1ccc(N=Nc2ccccc2)c2c1cccc2S(=O)(=O)O		$3.62e+02$	$5.62e+01$	$6.39e+03$	$2.94e-04$	$1.18e-03$	$2.79e+00$	6.51	*Yes*
449	70788-56-6	Clc1ccc(Cl)c(c1)C(=O)c1ccc(cc1)C(Cl)Cl		$1.25e+02$	$4.54e+02$	$9.72e+03$	$9.60e-05$	$8.10e-02$	$4.32e+00$	5.42	*No*
450	70788-61-3	Clc1cc(Cl)cc(c1)C(=O)c1ccc(C(Cl)Cl)c(c1)C(Cl)Cl		$3.13e+02$	$2.02e+03$	$6.95e+04$	$1.29e-05$	$5.70e-02$	$4.96e+00$	6.4	*No*

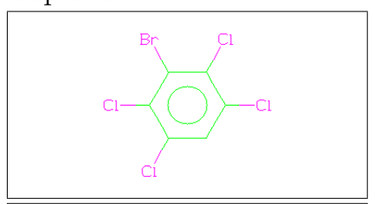
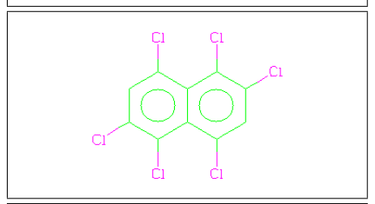
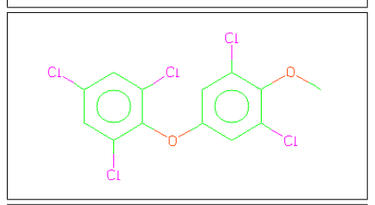
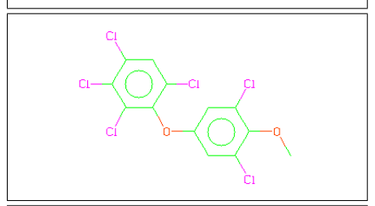
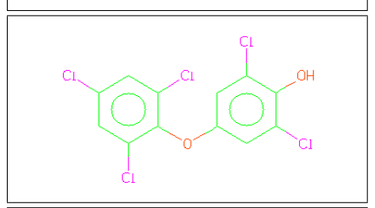
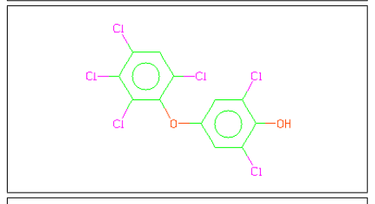
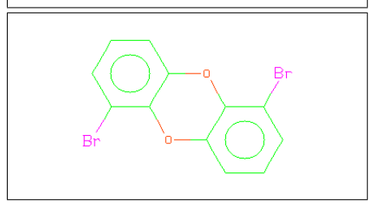
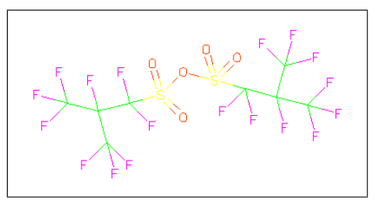
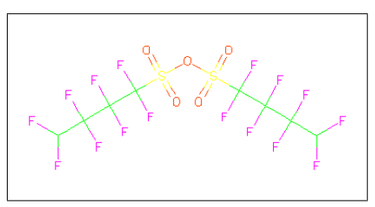
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
451	70865-38-2	`Cc1cccc(N=Nc2ccc(N=Nc3ccccc3)c3ccccc23)c1`		$1.06e+02$	$1.00e+01$	$1.65e+06$	$1.64e-05$	$6.57e-05$	$3.51e+00$	7.95	*No*
452	71215-80-0	`Brc1c(Br)c2oc(=O)c3ccc(cc3)c(=O)oc2c(Br)c1Br`		$1.19e+02$	$1.01e+04$	$2.64e+01$	$4.78e-04$	$4.50e-02$	$1.34e+01$	6.57	*No*
453	71216-04-1	`Brc1cc(Br)c(OC(=O)Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1`		$1.51e+03$	$3.12e+02$	$4.38e+04$	$7.22e-11$	$3.59e-05$	$2.77e+01$	10.33	*No*
454	71669-26-6	`Clc1c(Cl)cc2Oc3cccc(Cl)c3Oc2c1Cl`		$1.57e+02$	$7.64e+03$	$1.28e+04$	$6.99e-06$	$3.47e-04$	$9.03e+00$	6.655	*No*
455	71925-17-2	`Clc1cc2Oc3cc(Cl)c(Cl)c(Cl)c3Oc2c(Cl)c1`		$2.57e+02$	$7.76e+03$	$1.49e+04$	$1.09e-06$	$6.58e-05$	$1.33e+01$	6.98	*No*
456	72629-94-8	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.49e+03$	$1.00e+01$	$8.83e+06$	$3.34e-06$	$2.40e-04$	$2.06e+01$	8.16	*Yes*
457	72828-80-9	`CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCC`		$7.17e+01$	$1.04e+04$	$1.86e+03$	$7.49e-05$	$1.50e-02$	$2.40e+00$	6.59	*No*
458	73588-42-8	`Clc1cc(Cl)cc(c1)C(C)(Cl)CC(Cl)(Cl)Cl`		$4.70e+02$	$1.43e+04$	$2.10e+06$	$4.23e-06$	$2.30e-02$	$4.60e+00$	6.8	*No*
459	73881-45-5	`Ic1c(I)cc2ccccc2c1I`		$7.84e+01$	$4.51e+04$	$1.67e+03$	$2.34e-05$	$1.08e-03$	$4.87e+00$	6.67	*No*

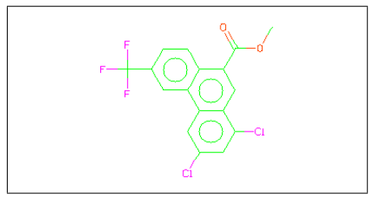
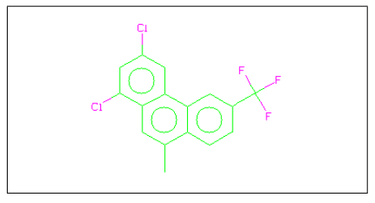
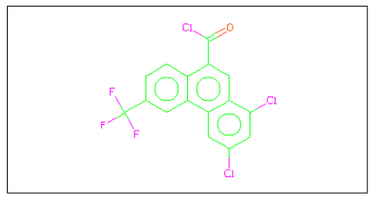
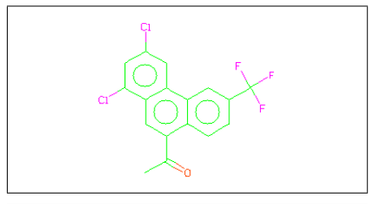
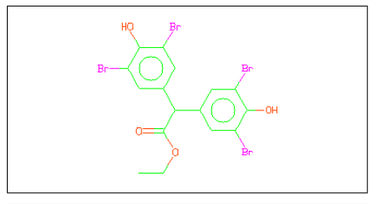
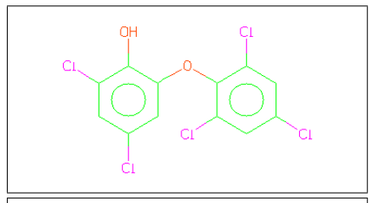
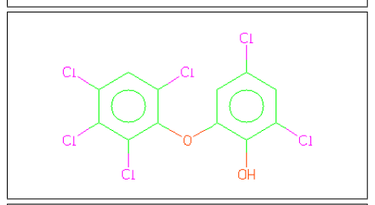
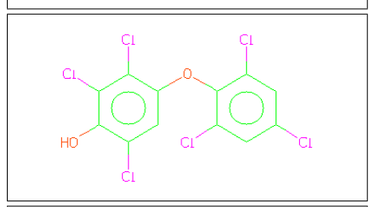
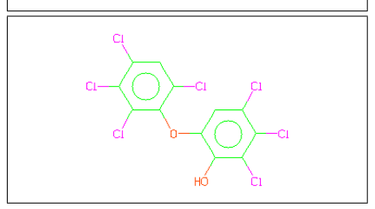
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
460	74298-69-4	`COc1c(Cl)cc(Cl)c2c(Cl)ccc(Cl)c12`		$1.29e+02$	$3.25e+03$	$5.58e+05$	$1.77e-04$	$6.00e-03$	$2.94e+00$	5.83	*No*
461	74298-91-2	`COc1c(Cl)cc(cc1Cl)c1ccc(Cl)cc1`		$8.71e+01$	$2.98e+03$	$1.06e+06$	$2.04e-04$	$7.00e-03$	$4.32e+00$	5.77	*No*
462	74298-92-3	`COc1ccc(cc1Cl)c1ccc(Cl)cc1Cl`		$8.71e+01$	$2.98e+03$	$1.06e+06$	$2.04e-04$	$7.00e-03$	$2.62e+00$	5.77	*No*
463	74472-52-9	`Clc1cc(Cl)c(c(Cl)c1)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$8.18e+02$	$5.92e+03$	$3.03e+06$	$2.20e-08$	$1.97e-06$	$8.67e+01$	8.91	*No*
464	75240-06-1	`FC1(F)C2(F)C(F)(F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C1(F)F`		$1.19e+03$	$1.34e+03$	$1.93e+04$	$1.45e-03$	$4.40e-02$	$1.00e+06$	5.24	*No*
465	76584-71-9	`Brc1cc(Br)c2Oc3cc(Br)cc(Br)c3Oc2c1`		$1.91e+02$	$4.81e+03$	$1.87e+04$	$5.50e-07$	$3.66e-05$	$7.36e+00$	7.9	*No*
466	76745-12-5	`Clc1cc(ccc1Cl)Sc1ccc(Cl)c(Cl)c1`		$1.30e+02$	$1.58e+04$	$2.71e+06$	$8.21e-06$	$4.02e-04$	$2.07e+00$	6.87	*No*
467	79780-39-5	`FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)O`		$1.31e+04$	$5.62e+01$	$5.87e+06$	*NA*	$4.73e-03$	$7.64e+01$	7.17	*Yes*
468	80246-33-9	`Brc1ccc2Oc3cc(Br)cc(Br)c3Oc2c1`		$1.11e+02$	$1.31e+04$	$9.68e+03$	$6.91e-06$	$3.53e-04$	$4.63e+00$	7.01	*No*

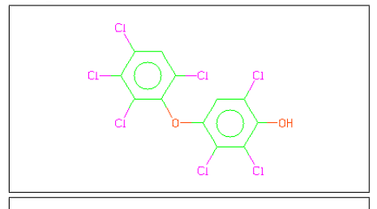
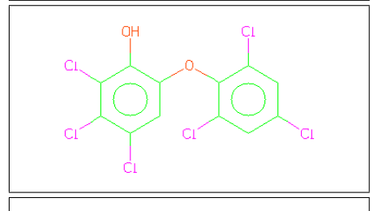
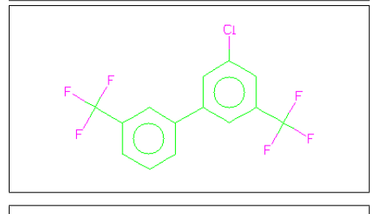
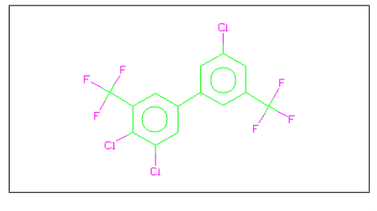
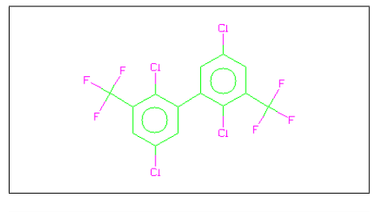
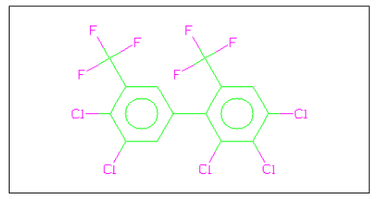
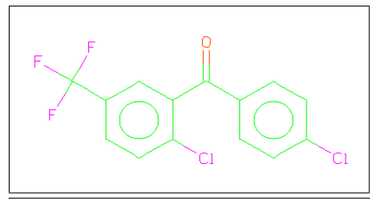
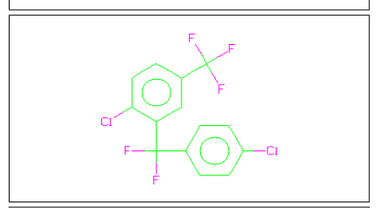
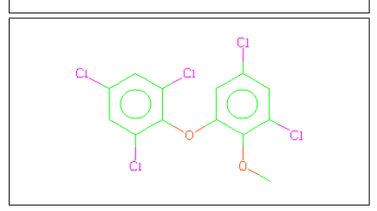
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
469	81012-95-5	`Clc1ccc(cc1)C(NC(=O)C)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl`		$5.01e+02$	$2.86e+03$	$4.56e+04$	NA	$7.49e-02$	$3.15e+00$	5.74	Yes
470	81686-42-2	`Clc1cc(C(C)C)c(Cl)c(Cl)c1C`		$8.43e+01$	$5.72e+03$	$2.18e+04$	$1.04e-04$	$4.00e-03$	$3.31e+00$	6.065	No
471	81686-43-3	`Clc1c(C)c(Cl)c(Cl)c(C(C)C)c1Cl`		$1.38e+02$	$1.42e+04$	$1.28e+05$	$1.68e-05$	$7.55e-04$	$4.01e+00$	6.685	No
472	83682-28-4	`ClC(C(Cl)C(C)(Cl)Cl)C(C)(Cl)Cl`		$3.48e+02$	$3.38e+03$	$2.78e+04$	$1.62e-04$	$6.00e-03$	$5.33e+01$	5.85	No
473	83682-29-5	`ClCC(Cl)(Cl)CCC(Cl)(Cl)CCl`		$3.48e+02$	$4.22e+03$	$4.23e+04$	$1.04e-04$	$4.00e-03$	$1.42e+01$	6	No
474	83682-31-9	`ClC(=C(Cl)C(C)(Cl)Cl)C(C)(Cl)Cl`		$3.45e+02$	$6.28e+03$	$5.21e+05$	$4.39e-05$	$3.00e-03$	$3.73e+00$	6.26	No
475	83682-40-0	`ClC(=C(CC(Cl)(Cl)Cl)C(Cl)(Cl)Cl)Cl`		$7.78e+02$	$6.44e+03$	$7.96e+05$	$4.96e-05$	$4.00e-03$	$2.85e+00$	6.28	No
476	83682-64-8	`ClCC(Cl)(Cl)C1(Cl)CCC(Cl)C(Cl)C1`		$3.84e+02$	$4.34e+03$	$1.01e+05$	$1.07e-04$	$4.00e-03$	$4.05e+00$	6.02	No
477	83682-70-6	`ClC(Cl)(C(C)(Cl)Cl)C(Cl)(Cl)Cl`		$6.96e+02$	$3.44e+03$	$6.70e+04$	$1.60e-04$	$6.00e-03$	$3.15e+02$	5.86	No

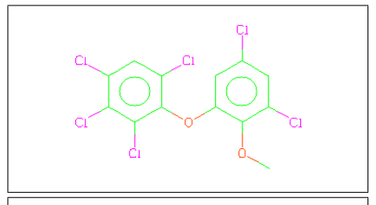
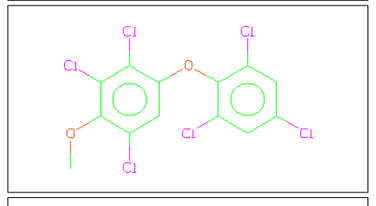
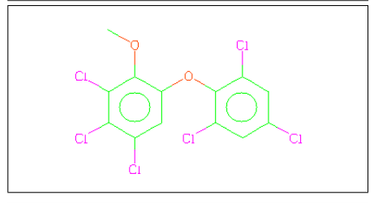
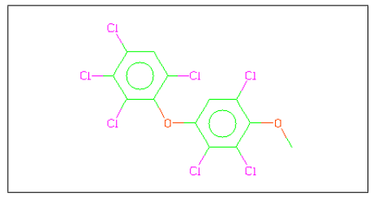
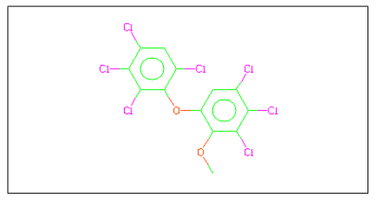
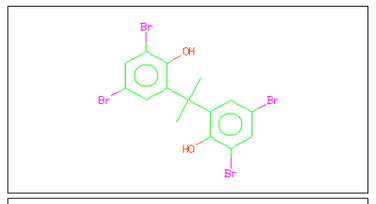
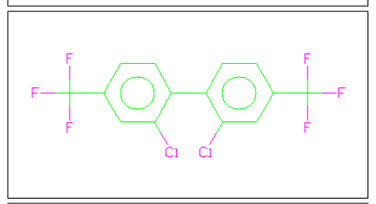
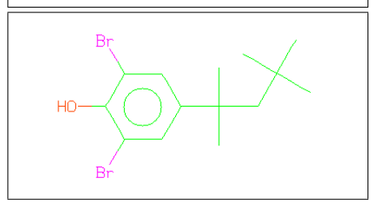
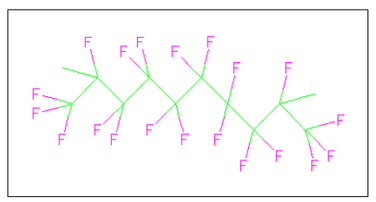
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
478	83929-71-9	`CCCC(=O)Oc1c(Br)c(Br)c(Br)c(Br)c1Br`		$1.94e+02$	$1.30e+04$	$6.14e+02$	NA	$5.34e-03$	$6.29e+00$	7.02	Yes
479	83992-71-6	`Clc1ccc(Oc2c(Cl)c(Cl)c c(Cl)c2Cl)c(Cl)c1Cl`		$5.89e+02$	$1.14e+04$	$4.17e+06$	$7.83e-07$	$4.94e-05$	$5.19e+01$	7.43	No
480	84604-89-7	`Clc1ccc(Cc2ccc(Cl)cc2C l)c(Cl)c1`		$1.38e+02$	$1.04e+04$	$1.18e+06$	NA	$7.87e-03$	$3.26e+00$	6.59	Yes
481	84604-90-0	`Clc1cccc(Cl)c1Cc1c(Cl) cccc1Cl`		$1.38e+02$	$1.04e+04$	$1.18e+06$	NA	$7.87e-03$	$3.26e+00$	6.59	Yes
482	84761-80-8	`Brc1cc2c(cc1Br)oc1ccc( Br)c(Br)c21`		$1.47e+02$	$9.76e+03$	$3.39e+03$	$3.57e-06$	$1.97e-04$	$5.48e+01$	7.27	No
483	84761-81-9	`Brc1ccc2oc3ccc(Br)c(Br )c3c2c1`		$8.55e+01$	$7.58e+03$	$1.16e+03$	$4.46e-05$	$1.89e-03$	$2.33e+01$	6.38	No
484	84761-82-0	`Brc1ccc2oc3cc(Br)c(Br) cc3c2c1`		$8.55e+01$	$7.58e+03$	$1.16e+03$	$4.46e-05$	$1.89e-03$	$2.33e+01$	6.38	No
485	85118-22-5	`Fc1ccc(cc1)C(Cl)c1ccc( cc1Br)C(F)(F)F`		$3.09e+02$	$4.01e+03$	$1.88e+05$	NA	$3.94e-02$	$4.38e+00$	5.97	Yes
486	85391-67-9	`Clc1cc(ccc1Cl)Oc1nc2c( Cl)cccc2s1`		$1.03e+02$	$5.38e+03$	$4.42e+03$	NA	$2.29e-02$	$2.62e+00$	6.16	Yes

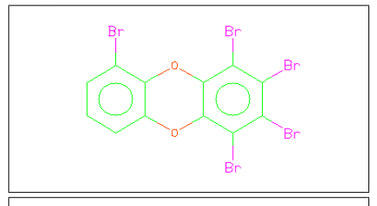
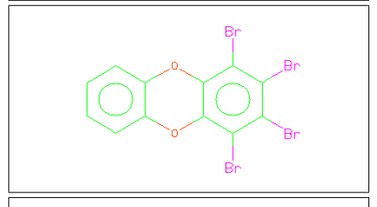
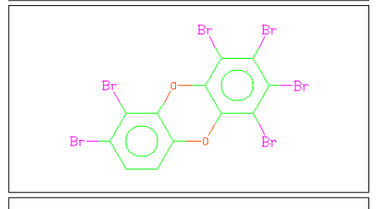
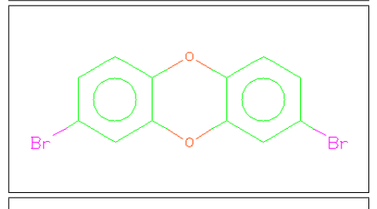
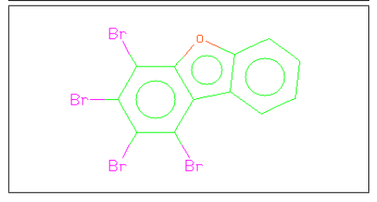
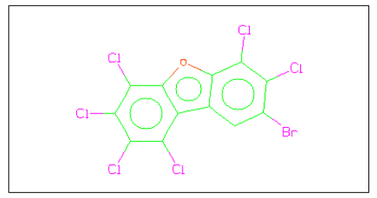
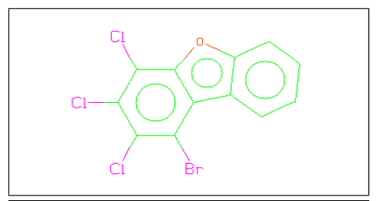
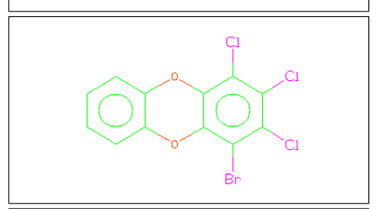
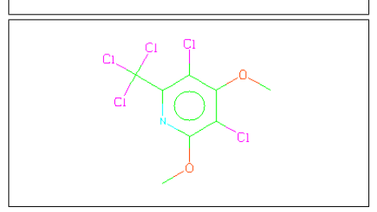
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
487	85720-79-2	FC(Cl)(C(F)(F)F)C(F)(Cl)C(F)(C(F)(F)F)C(F)(F)F		$2.95e+03$	$3.86e+03$	$5.33e+05$	NA	$4.26e-02$	$1.00e+06$	5.94	Yes
488	85721-08-0	Fc1ccc(cc1)C(=O)c1cc(ccc1Cl)C(F)(F)F		$2.09e+02$	$2.24e+02$	$8.48e+03$	$3.00e-03$	$7.10e-02$	$4.32e+00$	4.95	Yes
489	85721-09-1	Fc1ccc(cc1)C(=O)c1ccc(cc1Br)C(F)(F)F		$2.20e+02$	$3.26e+02$	$1.34e+04$	$1.39e-03$	$4.20e-02$	$4.46e+00$	5.2	Yes
490	85918-33-8	Clc1c(Cl)cc(Cl)c(Oc2ccccc2)c1Cl		$1.30e+02$	$3.52e+03$	$1.61e+04$	$2.08e-04$	$7.00e-03$	$6.21e+00$	5.835	No
491	311-89-7	FC(F)(N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F		$1.46e+05$	$3.44e+03$	$6.16e+06$	$2.43e-04$	$3.00e-03$	$1.00e+06$	8.2	Yes
492	88847-67-0	Clc1cc(Cl)c(Cl)cc1OP(=O)(C)Oc1cc(Cl)c(Cl)cc1Cl		$4.39e+02$	$1.46e+04$	$3.42e+06$	$3.90e-05$	$1.20e-02$	$1.88e+01$	6.82	No
493	89590-81-8	Clc1cccc(c1)c1cc(Cl)c(cc1Cl)c1cc(Cl)c(cc1Cl)c1cccc(Cl)c1		$5.49e+02$	$4.74e+02$	$2.97e+04$	$2.93e-11$	$5.10e-09$	$3.61e+00$	11.15	No
494	90077-76-2	Clc1c(Cl)ccc2c1C(=O)c1c2ccc(Cl)c1Cl		$1.32e+02$	$1.34e+03$	$5.42e+03$	$7.61e-05$	$3.00e-03$	$1.61e+01$	6.13	No
495	90077-77-3	Clc1ccc2c(c1Cl)C(=O)c1c2cc(Cl)c(Cl)c1Cl		$2.15e+02$	$3.56e+03$	$3.34e+04$	$1.19e-05$	$5.68e-04$	$2.48e+01$	6.77	No

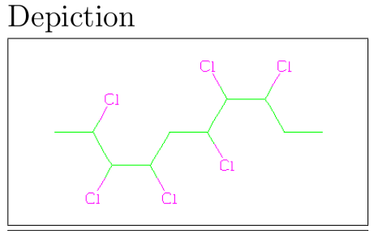
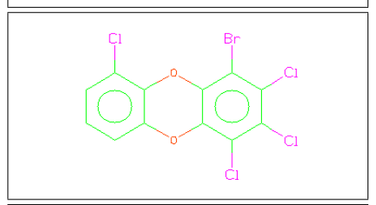
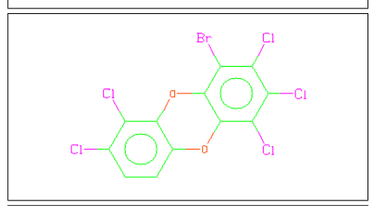
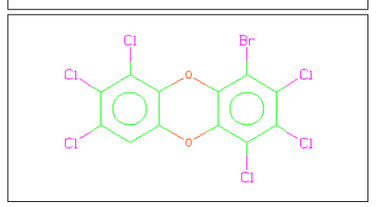
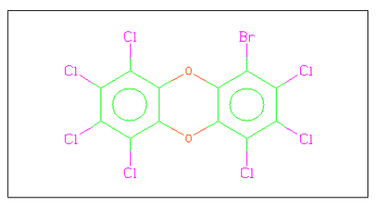
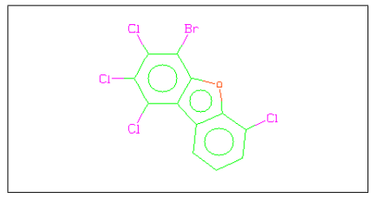
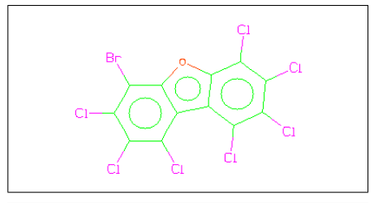
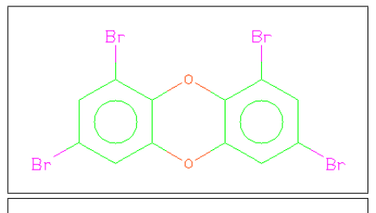
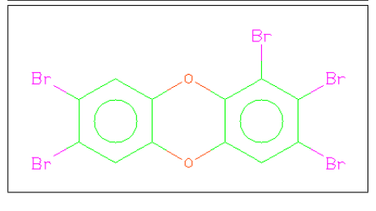
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
496	90077-78-4	`Clc1cc(Cl)c(Cl)c(Br)c1Cl`		$1.47e+02$	$1.86e+03$	$1.11e+04$	$5.36e-04$	$1.70e-02$	$2.07e+02$	5.46	*No*
497	90948-28-0	`Clc1cc(Cl)c2c(Cl)c(Cl)cc(Cl)c2c1Cl`		$2.77e+02$	$4.92e+04$	$1.92e+06$	$5.10e-06$	$2.63e-04$	$5.72e+01$	7.04	*No*
498	90985-94-7	`COc1c(Cl)cc(Oc2c(Cl)cc(Cl)cc2Cl)cc1Cl`		$2.74e+02$	$9.21e+03$	$4.35e+06$	$2.78e-05$	$1.22e-03$	$4.96e+00$	6.51	*No*
499	90985-96-9	`COc1c(Cl)cc(cc1Cl)Oc1c(Cl)cc(Cl)c(Cl)c1Cl`		$4.47e+02$	$1.11e+04$	$9.46e+06$	$4.29e-06$	$2.29e-04$	$6.64e+00$	7.16	*No*
500	90986-10-0	`Clc1cc(Cl)c(Oc2cc(Cl)c(O)c(Cl)c2)c(Cl)c1`		$2.13e+02$	$3.93e+03$	$9.46e+03$	$1.00e-02$	$5.00e-03$	$8.31e+00$	5.95	*No*
501	90986-11-1	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.36e+01$	6.6	*No*
502	91371-14-1	`Brc1cccc2Oc3c(Br)cccc3Oc12`		$6.49e+01$	$5.08e+03$	$2.11e+03$	$8.37e-05$	$3.00e-03$	$2.92e+00$	6.12	*No*
503	93894-52-1	`FC(F)(F)C(F)(C(F)(F)F)C(F)(F)S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.28e+04$	$4.07e+03$	$5.44e+06$	*NA*	$5.19e-04$	$1.00e+06$	8.05	*Yes*
504	93894-55-4	`FC(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)F`		$6.61e+02$	$1.25e+04$	$4.60e+05$	*NA*	$4.76e-03$	$1.73e+04$	7.06	*Yes*

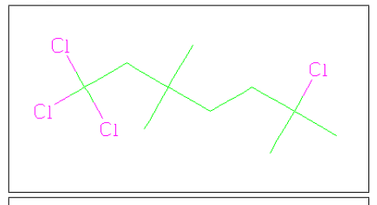
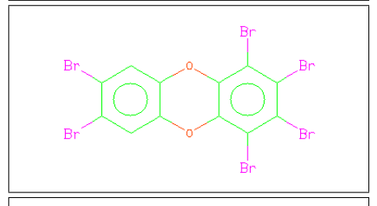
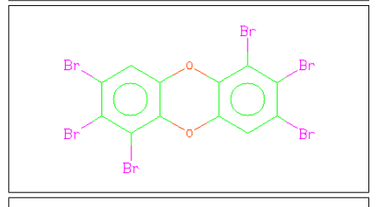
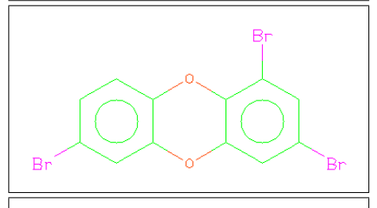
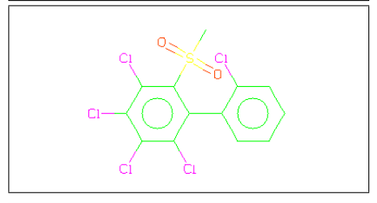
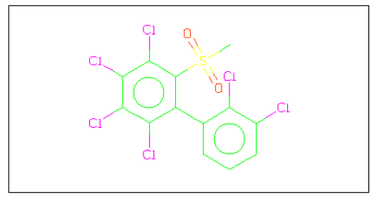
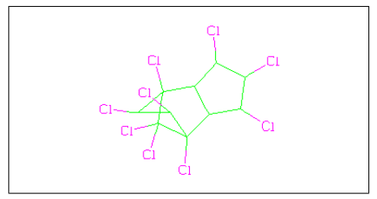
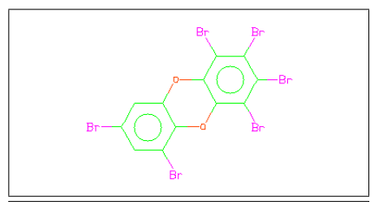
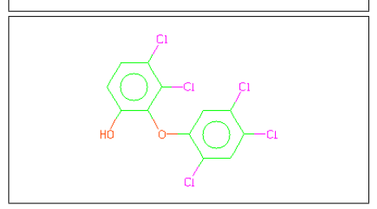
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
505	94133-65-0	`COC(=O)c1cc2c(Cl)cc(Cl)cc2c2cc(ccc12)C(F)(F)F`		$1.46e+02$	$3.73e+04$	$6.15e+02$	NA	$1.39e-02$	$3.13e+01$	6.43	Yes
506	94133-66-1	`Clc1cc(Cl)c2cc(C)c3ccc(cc3c2c1)C(F)(F)F`		$1.79e+02$	$5.18e+04$	$9.95e+04$	NA	$2.38e-03$	$1.10e+01$	7.14	Yes
507	94133-67-2	`Clc1cc(Cl)c2cc(C(=O)Cl)c3ccc(cc3c2c1)C(F)(F)F`		$1.89e+02$	$2.06e+04$	$2.44e+03$	NA	$3.44e-02$	$3.71e+01$	6.04	Yes
508	94133-68-3	`Clc1cc(Cl)c2cc(C(=O)C)c3ccc(cc3c2c1)C(F)(F)F`		$1.82e+02$	$7.67e+03$	$7.31e+03$	NA	$1.87e-02$	$2.74e+01$	6.28	Yes
509	94159-40-7	`CCOC(=O)C(c1cc(Br)c(O)c(Br)c1)c1cc(Br)c(O)c(Br)c1`		$1.60e+02$	$1.44e+04$	$2.48e+01$	$5.25e-05$	$1.60e-02$	$2.11e+00$	6.81	Yes
510	94888-09-2	`Clc1cc(Cl)c(Oc2cc(Cl)cc(Cl)c2O)c(Cl)c1`		$2.13e+02$	$3.93e+03$	$9.46e+03$	$1.00e-02$	$5.00e-03$	$8.31e+00$	5.95	No
511	94888-10-5	`Clc1cc(Oc2c(Cl)cc(Cl)c(Cl)c2Cl)c(O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.36e+01$	6.6	No
512	94888-11-6	`Clc1cc(Cl)c(Oc2cc(Cl)c(O)c(Cl)c2Cl)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.53e+01$	6.6	No
513	94888-12-7	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(Cl)c(Cl)c1O`		$5.68e+02$	$1.01e+04$	$2.92e+05$	$1.02e-03$	$2.83e-04$	$2.71e+01$	7.24	No

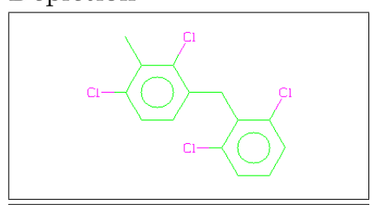
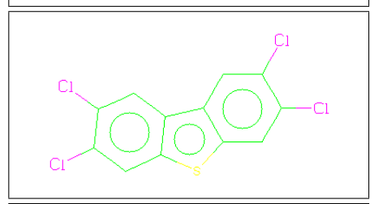
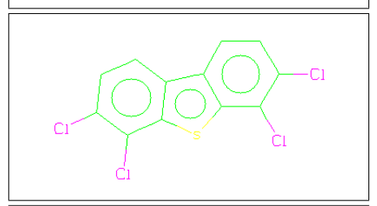
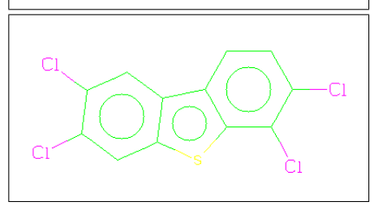
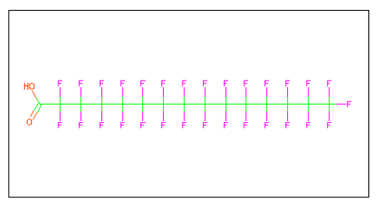
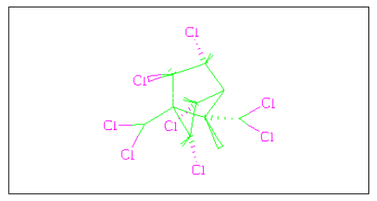
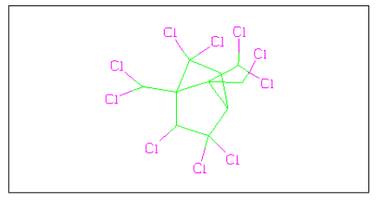
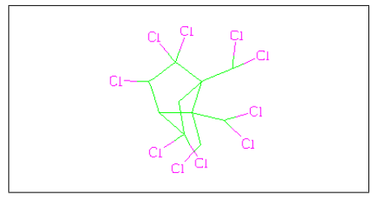
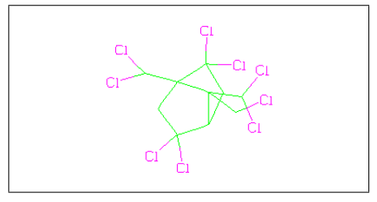
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
514	94888-13-8	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(O)c(Cl)c1Cl`		$5.68e+02$	$1.01e+04$	$2.92e+05$	$1.02e-03$	$2.83e-04$	$2.71e+01$	7.24	*No*
515	94897-81-1	`Clc1cc(Cl)c(Oc2cc(Cl)c(Cl)c(Cl)c2O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.53e+01$	6.6	*No*
516	95998-64-4	`Clc1cc(cc(c1)C(F)(F)F)c1cccc(c1)C(F)(F)F`		$2.63e+02$	$6.95e+03$	$3.44e+06$	$4.25e-05$	$1.77e-03$	$1.45e+01$	6.33	*No*
517	95998-66-6	`Clc1cc(cc(c1)C(F)(F)F)c1cc(Cl)c(Cl)c(c1)C(F)(F)F`		$7.03e+02$	$6.64e+03$	$1.17e+07$	$1.03e-06$	$6.29e-05$	$4.01e+01$	7.62	*No*
518	95998-67-7	`Clc1cc(c2cc(Cl)cc(c2Cl)C(F)(F)F)c(Cl)c(c1)C(F)(F)F`		$1.15e+03$	$3.21e+03$	$8.56e+06$	$1.58e-07$	$1.17e-05$	$9.68e+01$	8.26	*No*
519	95998-68-8	`Clc1cc(c(c2cc(Cl)c(Cl)c(c2)C(F)(F)F)c(Cl)c1Cl)C(F)(F)F`		$1.88e+03$	$1.55e+03$	$3.59e+06$	$2.42e-08$	$2.16e-06$	$2.11e+02$	8.91	*No*
520	95998-69-9	`Clc1ccc(cc1)C(=O)c1cc(ccc1Cl)C(F)(F)F`		$1.57e+02$	$4.41e+02$	$4.45e+04$	$7.00e-04$	$2.20e-02$	$7.12e+00$	5.4	*No*
521	95998-70-2	`Clc1ccc(cc1)C(F)(F)c1cc(ccc1Cl)C(F)(F)F`		$2.38e+02$	$8.49e+03$	$2.81e+06$	$2.99e-05$	$1.30e-03$	$5.41e+00$	6.46	*No*
522	97534-02-6	`COc1c(cc(Cl)cc1Cl)Oc1c(Cl)cc(Cl)cc1Cl`		$2.74e+02$	$9.21e+03$	$4.35e+06$	$2.78e-05$	$1.22e-03$	$4.96e+00$	6.51	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
523	97534-03-7	COc1c(cc(Cl)cc1Cl)Oc1c(Cl)cc(Cl)c(Cl)c1Cl		$4.47e+02$	$1.11e+04$	$9.46e+06$	$4.29e-06$	$2.29e-04$	$6.64e+00$	7.16	*No*
524	97534-04-8	COc1c(Cl)cc(Oc2c(Cl)cc(Cl)cc2Cl)c(Cl)c1Cl		$4.47e+02$	$1.11e+04$	$9.46e+06$	$4.29e-06$	$2.29e-04$	$7.41e+00$	7.16	*No*
525	97534-05-9	COc1c(Oc2c(Cl)cc(Cl)cc2Cl)cc(Cl)c(Cl)c1Cl		$4.47e+02$	$1.11e+04$	$9.46e+06$	$4.29e-06$	$2.29e-04$	$7.41e+00$	7.16	*No*
526	97534-06-0	COc1c(Cl)cc(Oc2c(Cl)cc(Cl)c(Cl)c2Cl)c(Cl)c1Cl		$7.31e+02$	$5.38e+03$	$1.06e+07$	$6.57e-07$	$4.24e-05$	$9.52e+00$	7.8	*No*
527	97534-07-1	COc1c(Oc2c(Cl)cc(Cl)c(Cl)c2Cl)cc(Cl)c(Cl)c1Cl		$7.31e+02$	$5.38e+03$	$1.06e+07$	$6.57e-07$	$4.24e-05$	$9.52e+00$	7.8	*No*
528	97890-15-8	Brc1cc(Br)c(O)c(c1)C(C)(C)c1cc(Br)cc(Br)c1O		$2.19e+02$	$6.35e+03$	$7.18e+02$	$1.40e-03$	$1.70e-02$	$3.62e+00$	7.2	*Yes*
529	99686-52-9	Clc1cc(ccc1c1ccc(cc1Cl)C(F)(F)F)C(F)(F)F		$4.30e+02$	$1.85e+04$	$8.95e+06$	$6.65e-06$	$3.36e-04$	$3.65e+01$	6.97	*No*
530	102127-40-2	Oc1c(Br)cc(cc1Br)C(C)(C)CC(C)(C)C		$1.09e+02$	$1.25e+04$	$1.04e+04$	$1.26e-03$	$3.68e-04$	$3.00e+00$	7.06	*No*
531	103188-55-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(C)(F)C(F)(F)F)C(F)(F)C(F)(F)C(C)(F)C(F)(F)F		$7.72e+03$	$2.78e+03$	$6.18e+06$	$1.34e-07$	$1.03e-05$	$3.93e+01$	8.39	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
532	103456-36-6	`Brc1c2Oc3cccc(Br)c3Oc2c(Br)c(Br)c1Br`		$3.27e+02$	$1.76e+03$	$1.20e+04$	$4.27e-08$	$3.70e-06$	$2.14e+01$	8.79	*No*
533	103456-39-9	`Brc1c2Oc3ccccc3Oc2c(Br)c(Br)c1Br`		$1.91e+02$	$4.81e+03$	$1.87e+04$	$5.50e-07$	$3.66e-05$	$1.33e+01$	7.9	*No*
534	103456-42-4	`Brc1ccc2Oc3c(Oc2c1Br)c(Br)c(Br)c(Br)c3Br`		$5.61e+02$	$6.46e+02$	$5.00e+03$	$3.26e-09$	$3.67e-07$	$6.09e+01$	9.68	*No*
535	105836-96-2	`Brc1ccc2Oc3ccc(Br)cc3Oc2c1`		$6.49e+01$	$5.08e+03$	$2.11e+03$	$8.37e-05$	$3.00e-03$	$2.92e+00$	6.12	*No*
536	106340-44-7	`Brc1c(Br)c(Br)c(Br)c2c1oc1ccccc21`		$1.47e+02$	$9.76e+03$	$3.39e+03$	$3.57e-06$	$1.97e-04$	$5.48e+01$	7.27	*No*
537	107207-47-6	`Brc1cc2c(oc3c(Cl)c(Cl)c(Cl)c(Cl)c23)c(Cl)c1Cl`		$5.54e+02$	$2.53e+03$	$5.35e+04$	$8.85e-08$	$6.97e-06$	$4.84e+02$	8.47	*No*
538	107227-56-5	`Clc1c(Cl)c2oc3ccccc3c2c(Br)c1Cl`		$1.27e+02$	$9.57e+03$	$4.24e+03$	$2.42e-05$	$1.07e-03$	$4.51e+01$	6.54	*No*
539	107227-75-8	`Brc1c2Oc3ccccc3Oc2c(Cl)c(Cl)c1Cl`		$1.65e+02$	$1.10e+04$	$4.56e+04$	$3.77e-06$	$2.02e-04$	$1.26e+01$	7.17	*No*
540	108030-77-9	`COc1nc(c(Cl)c(OC)c1Cl)C(Cl)(Cl)Cl`		$4.03e+02$	$5.14e+02$	$6.51e+03$	$5.82e-04$	$1.26e-01$	$4.92e+00$	4.61	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
541	108171-26-2	`CCC(C(C(CC(C(C(C)Cl)Cl)Cl)Cl)Cl)Cl`		$2.06e+02$	$7.03e+03$	$3.30e+04$	$4.46e-05$	$4.10e-02$	$5.07e+00$	6.34	*Yes*
542	109264-61-1	`Clc1cccc2Oc3c(Oc12)c(Br)c(Cl)c(Cl)c3Cl`		$2.70e+02$	$5.34e+03$	$1.05e+05$	$5.83e-07$	$3.78e-05$	$1.87e+01$	7.81	*No*
543	109264-65-5	`Clc1ccc2Oc3c(Oc2c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$4.41e+02$	$2.58e+03$	$1.19e+05$	$8.96e-08$	$7.02e-06$	$5.15e+01$	8.45	*No*
544	109264-67-7	`Clc1c(Cl)cc2Oc3c(Oc2c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$7.21e+02$	$1.25e+03$	$8.66e+04$	$1.37e-08$	$1.30e-06$	$7.77e+01$	9.1	*No*
545	109264-69-9	`Clc1c2Oc3c(Oc2c(Cl)c(Cl)c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$1.18e+03$	$6.02e+02$	$4.92e+04$	$2.07e-09$	$2.38e-07$	$1.99e+02$	9.74	*No*
546	109302-36-5	`Clc1c(Br)c2oc3c(Cl)ccc c3c2c(Cl)c1Cl`		$2.07e+02$	$1.08e+04$	$1.90e+04$	$3.76e-06$	$2.02e-04$	$9.95e+01$	7.18	*No*
547	109302-40-1	`Clc1c(Cl)c2oc3c(Br)c(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl`		$9.06e+02$	$1.22e+03$	$4.24e+04$	$1.35e-08$	$1.28e-06$	$1.07e+03$	9.12	*No*
548	109333-30-4	`Brc1cc2Oc3cc(Br)cc(Br)c3Oc2c(Br)c1`		$1.91e+02$	$4.81e+03$	$1.87e+04$	$5.50e-07$	$3.66e-05$	$7.36e+00$	7.9	*No*
549	109333-34-8	`Brc1cc2Oc3c(Oc2cc1Br)cc(Br)c(Br)c3Br`		$3.27e+02$	$1.76e+03$	$1.20e+04$	$4.27e-08$	$3.70e-06$	$2.65e+01$	8.79	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
550	109749-69-1	`CC(C)(Cl)CCC(C)(C)CC(Cl)(Cl)Cl`		$2.62e+02$	$1.12e+04$	$2.37e+05$	$1.42e-05$	$6.50e-04$	$3.29e+00$	6.64	*No*
551	110999-44-5	`Brc1cc2Oc3c(Oc2cc1Br)c(Br)c(Br)c(Br)c3Br`		$5.61e+02$	$6.46e+02$	$5.00e+03$	$3.26e-09$	$3.67e-07$	$6.09e+01$	9.68	*No*
552	110999-45-6	`Brc1cc2Oc3c(cc(Br)c(Br)c3Br)Oc2c(Br)c1Br`		$5.61e+02$	$6.46e+02$	$5.00e+03$	$3.26e-09$	$3.67e-07$	$4.34e+01$	9.68	*No*
553	110999-49-0	`Brc1ccc2Oc3c(cc(Br)cc3Br)Oc2c1`		$1.11e+02$	$1.31e+04$	$9.68e+03$	$6.91e-06$	$3.53e-04$	$4.63e+00$	7.01	*No*
554	112815-67-5	`Clc1ccccc1c1c(Cl)c(Cl)c(Cl)c(Cl)c1S(=O)(=O)C`		$2.53e+02$	$2.13e+03$	$1.53e+05$	$5.62e-04$	$1.90e-02$	$7.77e+00$	5.55	*No*
555	112815-68-6	`Clc1cccc(c1Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1S(=O)(=O)C`		$4.13e+02$	$5.67e+03$	$1.17e+06$	$8.62e-05$	$3.00e-03$	$8.82e+00$	6.19	*No*
556	115384-94-6	`ClC1C(Cl)C2C(C1Cl)C1(Cl)C(Cl)C(Cl)C2(Cl)C1(Cl)Cl`		$2.24e+03$	$4.43e+03$	$1.33e+06$	$1.43e-04$	$5.00e-03$	$7.03e+00$	6.03	*No*
557	116490-11-0	`Brc1cc(Br)c2Oc3c(Oc2c1)c(Br)c(Br)c(Br)c3Br`		$5.61e+02$	$6.46e+02$	$5.00e+03$	$3.26e-09$	$3.67e-07$	$3.41e+01$	9.68	*No*
558	119036-18-9	`Clc1cc(Cl)c(Cl)cc1Oc1c(O)ccc(Cl)c1Cl`		$2.13e+02$	$3.93e+03$	$9.46e+03$	$1.00e-02$	$5.00e-03$	$2.74e+00$	5.95	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
559	121107-47-9	`Cc1c(Cl)ccc(Cc2c(Cl)ccc2Cl)c1Cl`		$1.66e+02$	$1.06e+04$	$1.60e+06$	$3.55e-06$	$1.88e-04$	$2.90e+00$	7.17	*No*
560	133513-17-4	`Clc1cc2sc3cc(Cl)c(Cl)cc3c2cc1Cl`		$1.29e+02$	$1.31e+04$	$9.26e+03$	$1.19e-05$	$5.63e-04$	$3.13e+01$	6.74	*No*
561	133513-18-5	`Clc1c(Cl)ccc2c1sc1c(Cl)c(Cl)ccc21`		$1.29e+02$	$1.31e+04$	$9.26e+03$	$1.19e-05$	$5.63e-04$	$3.13e+01$	6.74	*No*
562	133513-19-6	`Clc1cc2c(cc1Cl)sc1c(Cl)c(Cl)ccc21`		$1.29e+02$	$1.31e+04$	$9.26e+03$	$1.19e-05$	$5.63e-04$	$3.13e+01$	6.74	*No*
563	141074-63-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.61e+04$	$3.16e+00$	$1.17e+06$	$6.61e-08$	$7.06e-06$	$2.06e+01$	9.5	*No*
564	142534-71-2	`Cl[C@@H]1C2[C@@H](Cl)[C@H](Cl)C(C(Cl)Cl)([C@H]1Cl)[C@@]2(C)C(Cl)Cl`		$1.01e+03$	$2.04e+03$	$2.10e+05$	$1.55e-04$	$6.00e-03$	$5.88e+00$	5.75	*No*
565	151183-19-6	`ClCC1(C(Cl)Cl)C2CC(Cl)(Cl)C1(C(Cl)Cl)C(Cl)C2(Cl)Cl`		$5.02e+03$	$1.12e+04$	$2.72e+06$	$5.40e-07$	$3.58e-05$	$6.09e+00$	7.27	*No*
566	151183-20-9	`ClCC1(C(Cl)Cl)C2C(Cl)C(Cl)(Cl)C1(CC2(Cl)Cl)C(Cl)Cl`		$5.02e+03$	$4.84e+03$	$6.39e+06$	$5.40e-07$	$3.58e-05$	$6.93e+00$	7.9	*No*
567	154159-06-5	`ClCC1(C(Cl)Cl)C2CC(Cl)(Cl)C1(CC2(Cl)Cl)C(Cl)Cl`		$3.26e+03$	$3.98e+03$	$2.88e+05$	$8.67e-07$	$5.46e-05$	$5.96e+00$	6.84	*No*

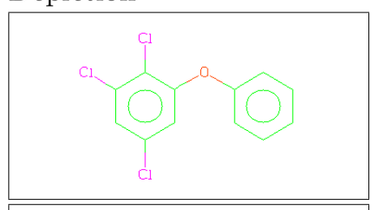
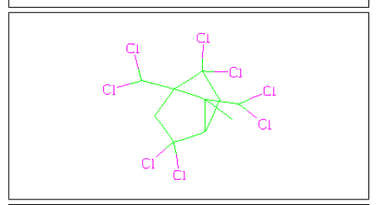
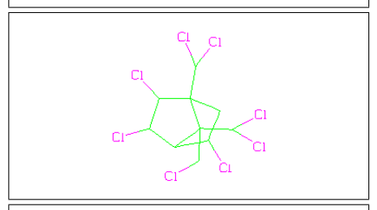
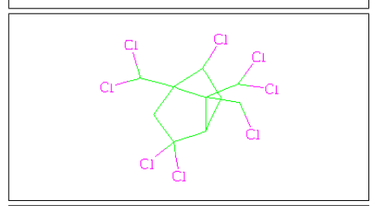
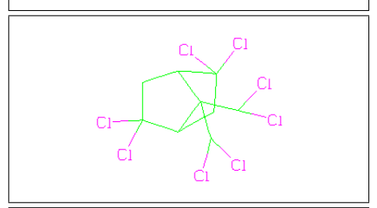
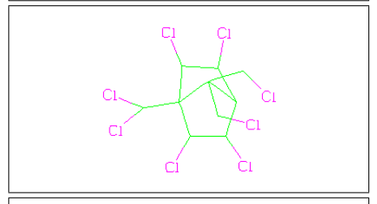
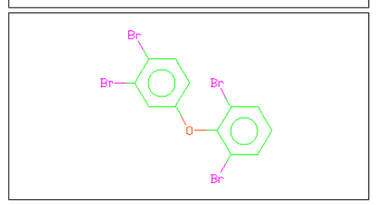
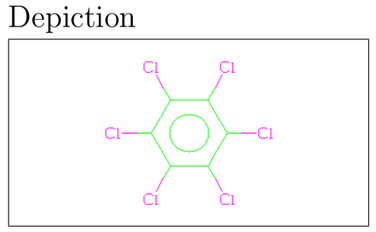
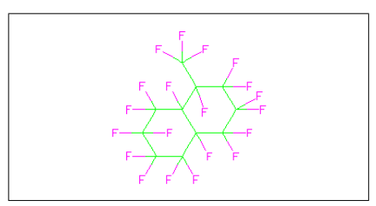
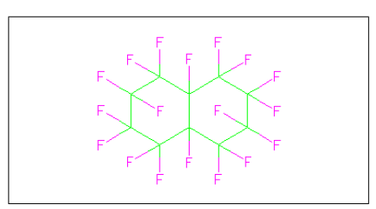
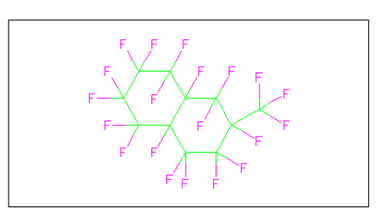
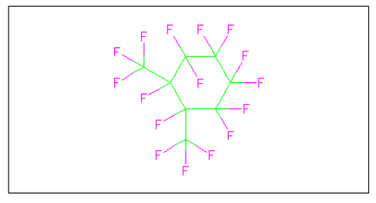
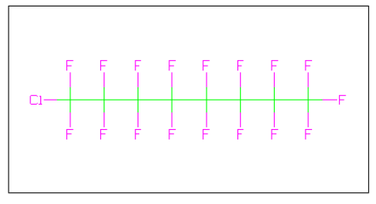
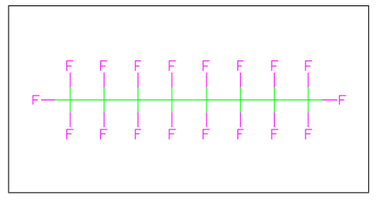
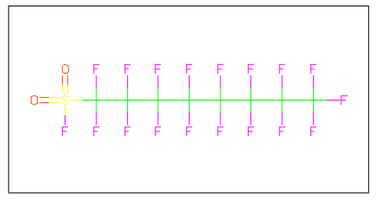
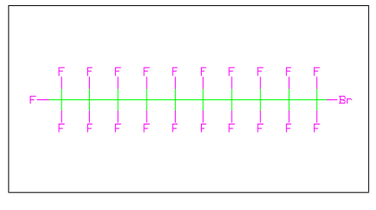
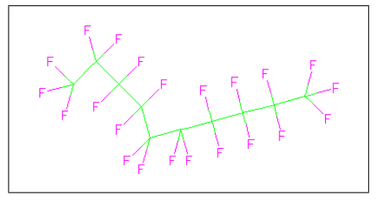
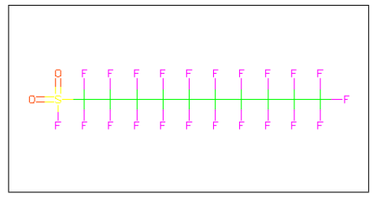
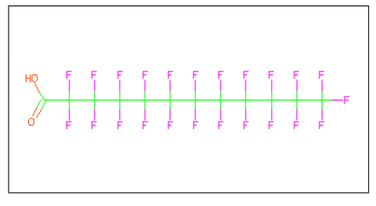
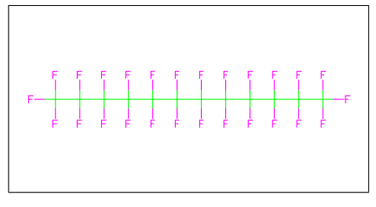
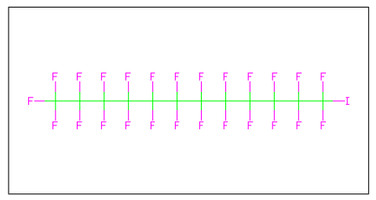
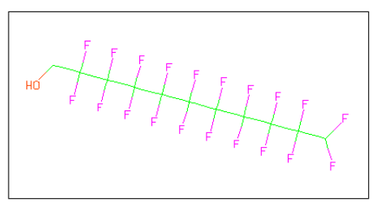
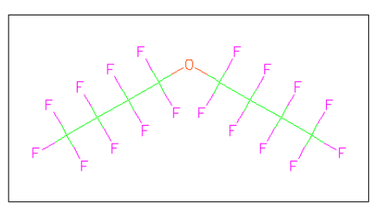
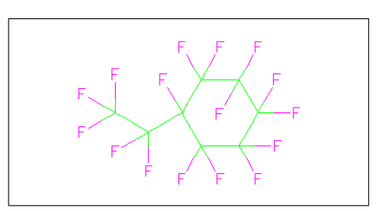
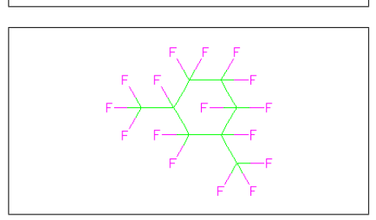
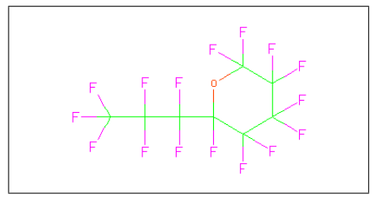
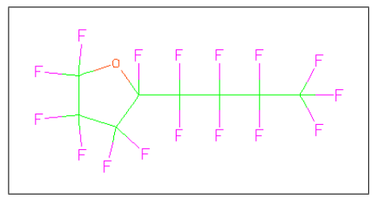
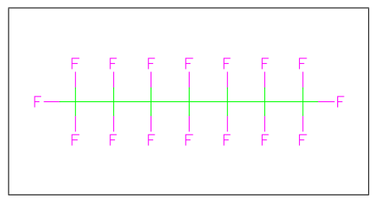
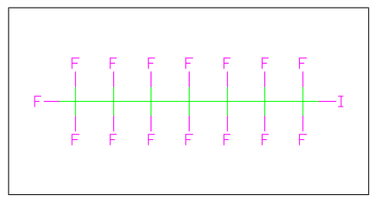
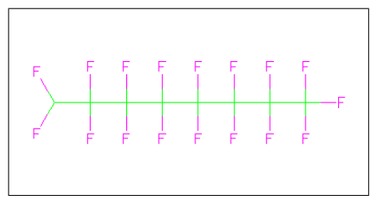
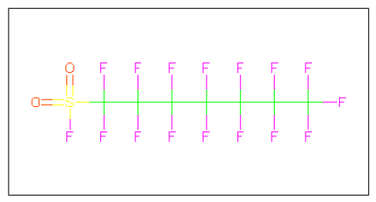
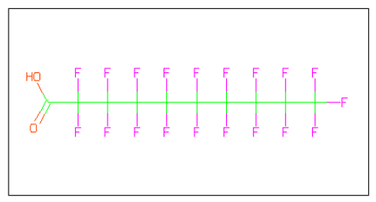
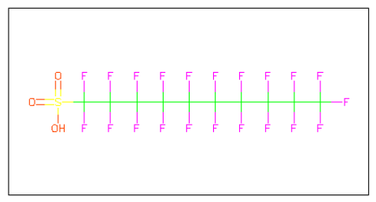
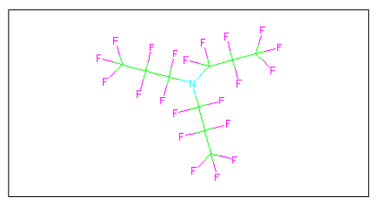
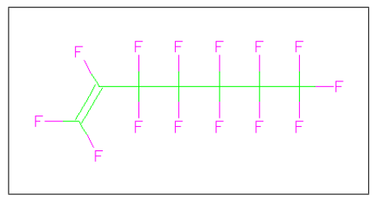
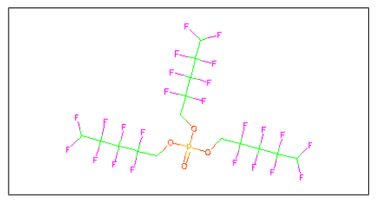
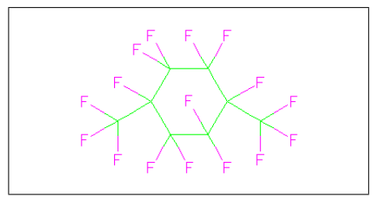
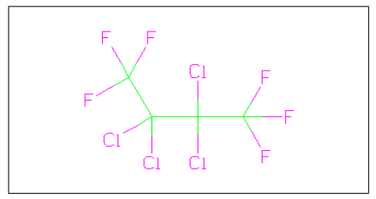
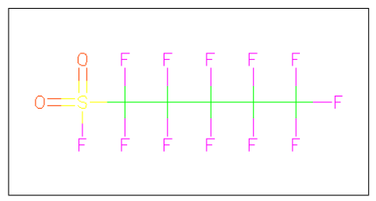
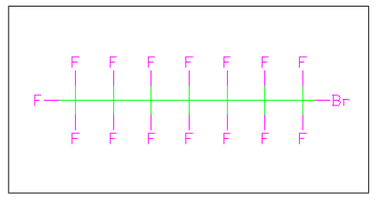
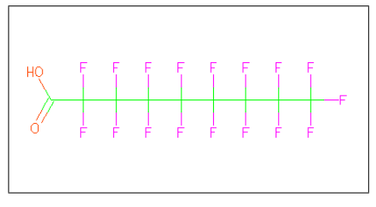
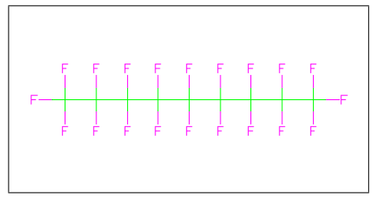
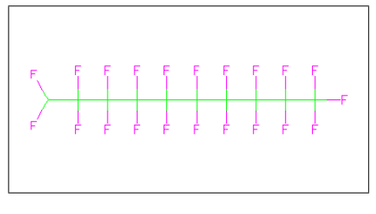
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
568	162853-24-9	`Clc1cc(Oc2ccccc2)c(Cl)c(Cl)c1`		$7.94e+01$	$2.37e+03$	$6.95e+03$	$1.30e-03$	$3.80e-02$	$3.84e+00$	5.38	*No*
569	165820-15-5	`ClC(Cl)C12CC(Cl)(Cl)C(CC1(Cl)Cl)C2(C)C(Cl)Cl`		$2.11e+03$	$3.63e+03$	$1.98e+05$	$1.73e-06$	$1.01e-04$	$7.02e+00$	6.68	*No*
570	165820-16-6	`ClCC1(C(Cl)Cl)C2C(Cl)CC1(C(Cl)Cl)C(Cl)C2Cl`		$1.01e+03$	$1.23e+03$	$4.58e+04$	$1.24e-04$	$5.00e-03$	$4.04e+00$	5.62	*No*
571	165820-17-7	`ClCC1(C(Cl)Cl)C2CC(Cl)C1(CC2(Cl)Cl)C(Cl)Cl`		$1.46e+03$	$2.89e+03$	$1.66e+05$	$1.31e-05$	$6.28e-04$	$4.13e+00$	6.27	*No*
572	165820-18-8	`ClC(Cl)C1(C(Cl)Cl)C2CC(Cl)(Cl)C1CC2(Cl)Cl`		$1.38e+03$	$3.07e+03$	$1.98e+05$	$6.62e-06$	$3.38e-04$	$6.45e+00$	6.4	*No*
573	166021-27-8	`ClCC1(CCl)C2C(Cl)C(Cl)C1(C(Cl)Cl)C(Cl)C2Cl`		$1.01e+03$	$2.20e+03$	$2.47e+05$	$1.24e-04$	$5.00e-03$	$4.91e+00$	5.81	*No*
574	189084-62-6	`Brc1cccc(Br)c1Oc1ccc(Br)c(Br)c1`		$1.63e+02$	$1.36e+04$	$5.72e+05$	$1.66e-05$	$7.90e-04$	$1.06e+01$	6.77	*No*

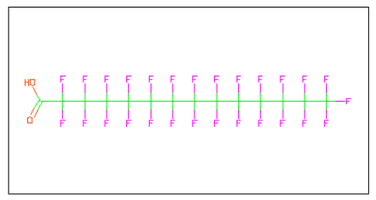
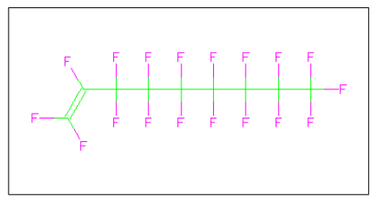
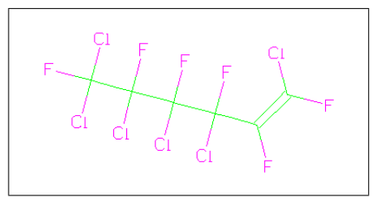
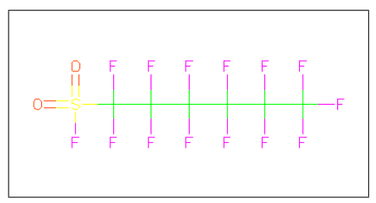
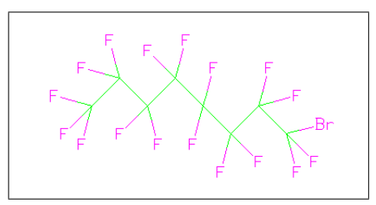
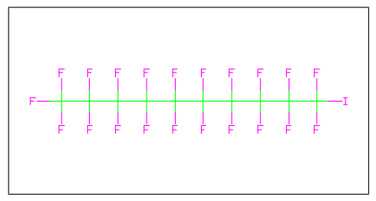
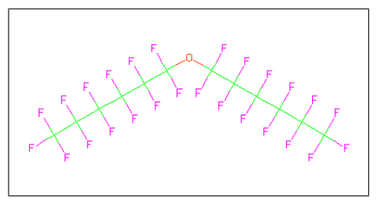
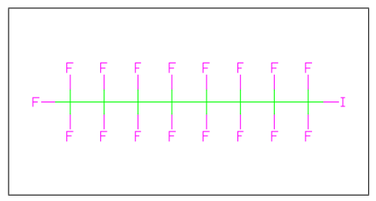
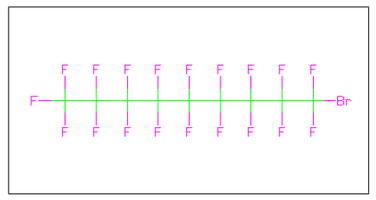
Table S3: Chemicals strongly exceeding the Annex D criteria of the Stockholm Convention ("very-POP group")

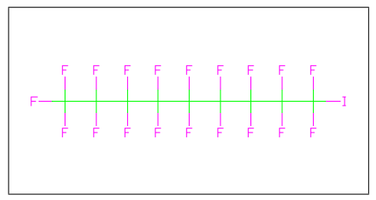
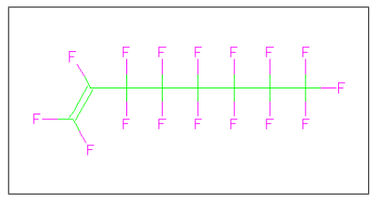
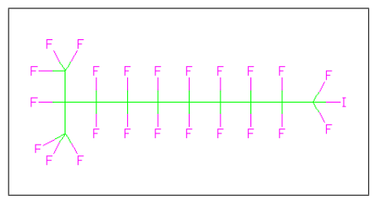
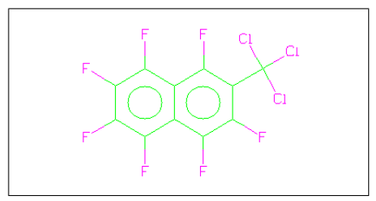
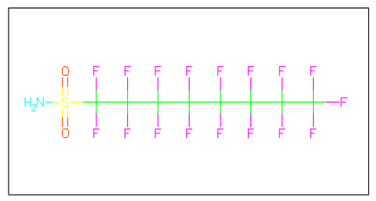
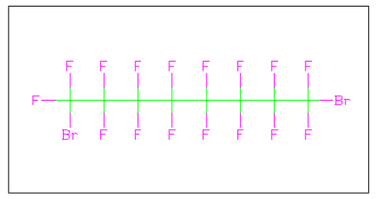
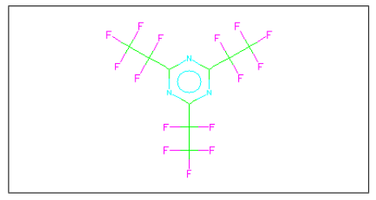
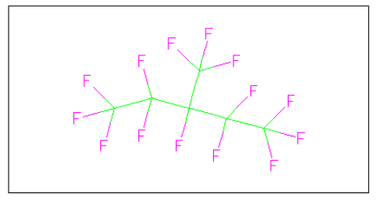
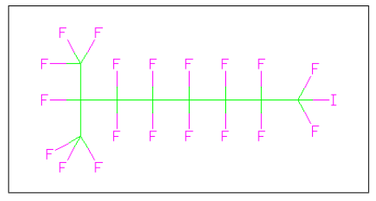
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
1	118-74-1	`Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.29e+02$	$1.33e+04$	$7.91e+05$	$1.54e-04$	$2.00e-03$	$1.58e+02$	5.795	*Yes*
2	306-92-3	`FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(C1(F)F)C(F)(F)C(F)(F)C(F)(F)C2(F)C(F)(F)F`		$6.17e+03$	$8.63e+03$	$2.37e+06$	$4.35e-05$	$1.89e-03$	$1.00e+06$	6.47	*Yes*
3	306-94-5	`FC1(F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C2(F)C1(F)F`		$2.09e+03$	$2.59e+03$	$1.33e+05$	$4.35e-04$	$1.50e-02$	$1.00e+06$	5.68	*Yes*
4	306-95-6	`FC1(F)C2(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C2(F)C(F)(F)C(F)(F)C1(F)F`		$6.17e+03$	$1.33e+04$	$5.44e+06$	$8.67e-06$	$4.41e-04$	$1.00e+06$	7	*Yes*
5	306-98-9	`FC1(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(C(F)(F)F)C1(F)F`		$2.24e+03$	$1.93e+03$	$3.03e+04$	$6.74e-04$	$2.20e-02$	$1.00e+06$	5.49	*Yes*
6	307-33-5	`FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Cl)C(F)(F)C(F)(F)F`		$2.21e+03$	$8.80e+03$	$2.09e+06$	$3.71e-05$	$1.62e-03$	$1.00e+06$	6.48	*Yes*
7	307-34-6	`FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.59e+03$	$5.47e+03$	$1.16e+06$	$9.26e-05$	$4.00e-03$	$1.00e+06$	6.17	*Yes*
8	307-35-7	`FS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.97e+03$	$5.19e+03$	$4.73e+06$	$3.43e-04$	$4.00e-03$	$1.00e+06$	7.84	*Yes*
9	307-43-7	`FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br`		$5.67e+03$	$4.76e+03$	$6.99e+06$	$6.42e-07$	$4.28e-05$	$1.00e+06$	7.91	*Yes*

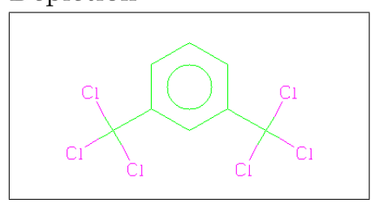
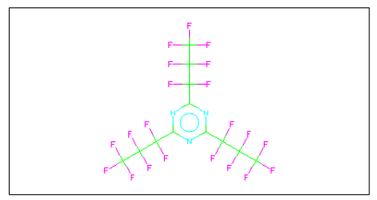
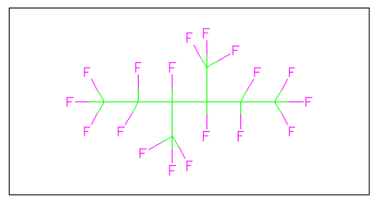
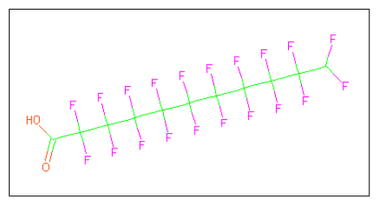
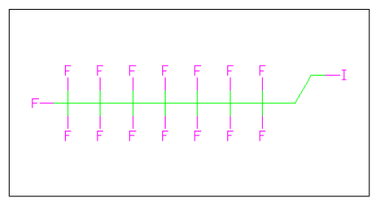
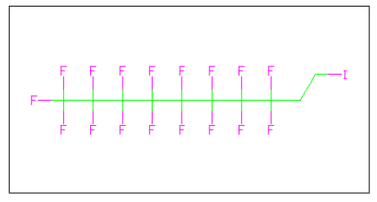
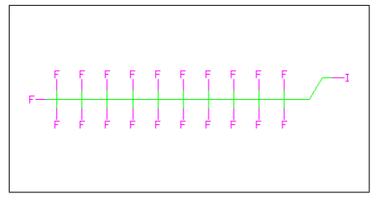
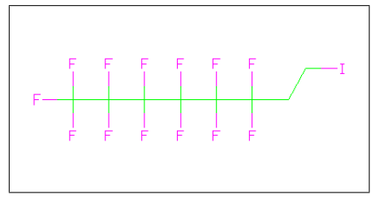
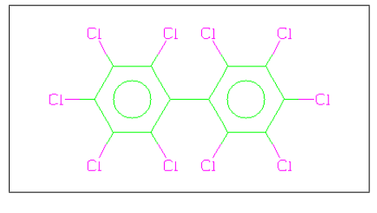
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
10	307-45-9	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$7.96e+03$	$7.50e+03$	$9.73e+06$	$1.96e-06$	$1.16e-04$	$1.00e+06$	7.51	*No*
11	307-51-7	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)F		$6.03e+03$	$1.15e+03$	$1.56e+06$	$5.91e-05$	$3.95e-04$	$1.00e+06$	9.17	*Yes*
12	307-55-1	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$4.85e+03$	$5.62e+01$	$1.01e+07$	$2.35e-05$	$1.39e-03$	$2.06e+01$	7.49	*Yes*
13	307-59-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.44e+04$	$1.66e+03$	$3.86e+06$	$4.00e-08$	$3.51e-06$	$1.00e+06$	8.85	*Yes*
14	307-60-8	FC(F)(I)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.19e+04$	$6.59e+02$	$5.49e+05$	$3.90e-09$	$4.37e-07$	$1.00e+06$	9.66	*Yes*
15	307-70-0	OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.43e+03$	$4.13e+03$	$1.73e+05$	$1.97e-04$	$7.00e-03$	$5.37e+01$	5.99	*Yes*
16	308-48-5	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.80e+03$	$1.06e+04$	$2.70e+06$	$3.00e-03$	$4.40e-02$	$1.00e+06$	6.61	*No*
17	335-21-7	FC1(F)C(F)(F)C(F)(F)C(F)(C(F)(F)C(F)(F)F)C(F)(F)C1(F)F		$1.33e+03$	$2.52e+03$	$3.43e+04$	$3.98e-04$	$1.40e-02$	$1.00e+06$	5.66	*No*
18	335-27-3	FC1(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C1(F)F		$2.24e+03$	$4.34e+03$	$1.78e+05$	$1.34e-04$	$5.00e-03$	$1.00e+06$	6.02	*Yes*

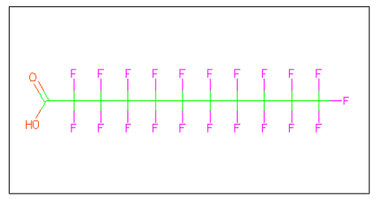
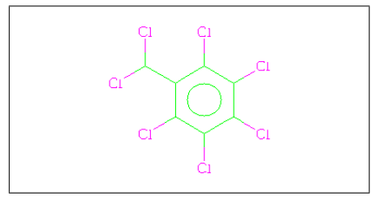
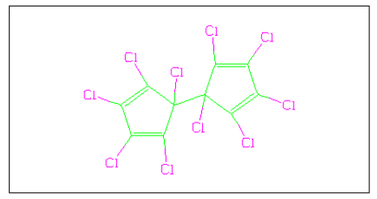
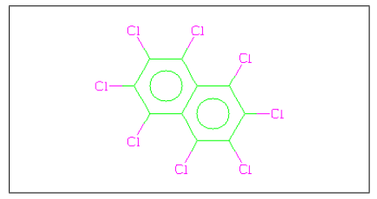
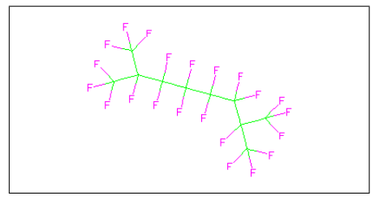
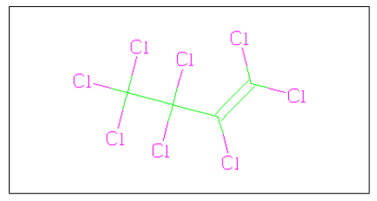
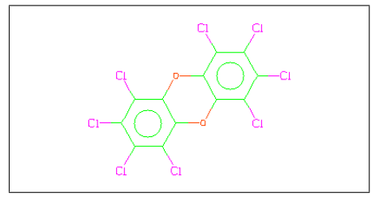
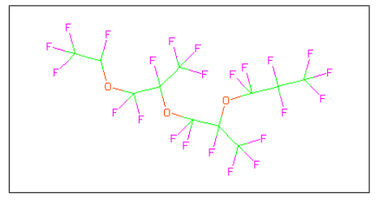
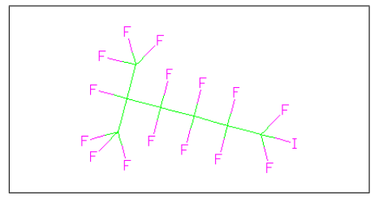
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
19	335-35-3	FC(F)(C(F)(F)F)C(F)(F)C1(F)OC(F)(F)C(F)(F)C(F)(F)C1(F)F		$1.43e+03$	$3.58e+03$	$5.57e+04$	$8.00e-03$	$1.51e-01$	$1.00e+06$	5.89	*Yes*
20	335-36-4	FC(F)(C(F)(F)C1(F)OC(F)(F)C(F)(F)C1(F)F)C(F)(F)C(F)(F)F		$1.43e+03$	$5.12e+03$	$1.19e+05$	$5.00e-03$	$9.80e-02$	$1.00e+06$	6.13	*Yes*
21	335-57-9	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F		$1.48e+03$	$1.98e+03$	$1.02e+05$	$6.26e-04$	$2.00e-02$	$1.00e+06$	5.5	*Yes*
22	335-58-0	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)F		$1.33e+03$	$6.85e+03$	$1.01e+05$	$6.68e-05$	$3.00e-03$	$1.00e+06$	6.32	*Yes*
23	335-65-9	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$9.93e+02$	$2.17e+03$	$8.92e+04$	$5.62e-04$	$1.90e-02$	$3.45e+04$	5.56	*Yes*
24	335-71-7	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)F		$1.12e+03$	$1.10e+04$	$2.68e+06$	$8.14e-04$	$1.50e-02$	$1.00e+06$	7.17	*Yes*
25	335-76-2	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.58e+03$	$5.62e+01$	$1.24e+06$	$1.15e-03$	$4.50e-02$	$2.06e+01$	6.15	*Yes*
26	335-77-3	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)O		$4.28e+03$	$1.00e+01$	$1.79e+05$	$4.00e-03$	$1.27e-01$	$7.64e+01$	5.83	*Yes*
27	338-83-0	FC(F)(C(F)(F)F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F		$1.35e+04$	$5.65e+03$	$4.38e+05$	$7.00e-03$	$5.70e-02$	$1.00e+06$	6.19	*Yes*

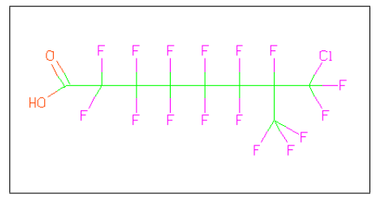
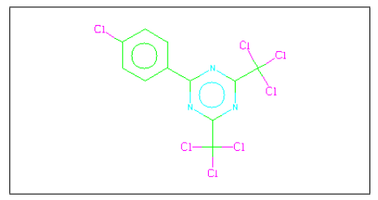
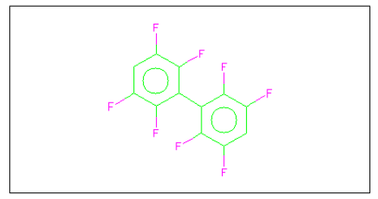
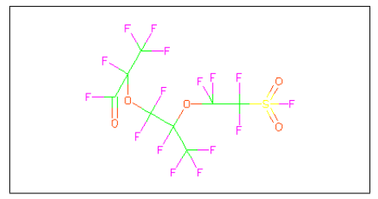
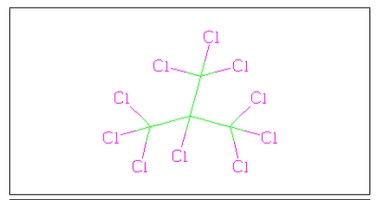
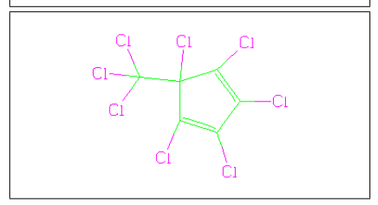
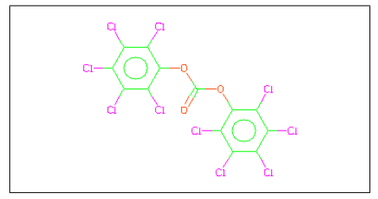
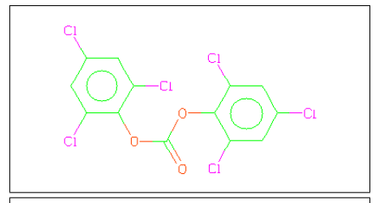
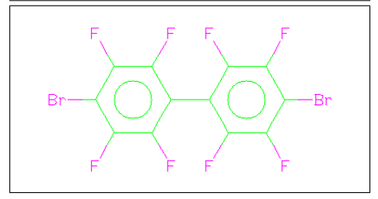
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
28	355-63-5	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)F		$3.63e+02$	$1.07e+03$	$2.62e+04$	$1.93e-03$	$5.60e-02$	$1.38e+01$	5.1	*Yes*
29	355-86-2	FC(F)C(F)(F)C(F)(F)C(F)(F)COP(=O)(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F		$3.22e+03$	$1.57e+03$	$8.58e+05$	*NA*	$4.56e-03$	$1.03e+01$	7.21	*Yes*
30	374-77-6	FC1(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C1(F)C(F)(F)F		$2.24e+03$	$9.72e+03$	$7.87e+05$	$2.68e-05$	$1.19e-03$	$1.00e+06$	6.55	*No*
31	375-34-8	FC(F)(F)C(Cl)(Cl)C(Cl)(Cl)C(F)(F)F		$1.18e+03$	$1.55e+03$	$2.95e+04$	$7.96e-04$	$2.50e-02$	$1.00e+06$	5.34	*Yes*
32	375-81-5	FS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.66e+02$	$3.25e+03$	$4.10e+04$	$4.00e-03$	$1.43e-01$	$1.00e+06$	5.83	*Yes*
33	375-88-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)F		$1.05e+03$	$3.65e+03$	$1.57e+05$	$2.13e-04$	$8.00e-03$	$1.00e+06$	5.9	*Yes*
34	375-95-1	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$9.02e+02$	$1.00e+01$	$1.12e+05$	$8.00e-03$	$2.56e-01$	$2.06e+01$	5.48	*Yes*
35	375-96-2	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$4.54e+03$	$1.51e+04$	$5.39e+06$	$1.35e-05$	$6.57e-04$	$1.00e+06$	6.84	*No*
36	375-97-3	FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.05e+03$	$1.66e+04$	$4.95e+06$	*NA*	$6.55e-03$	$3.45e+04$	6.9	*Yes*

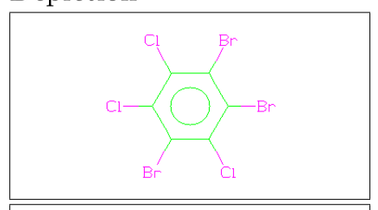
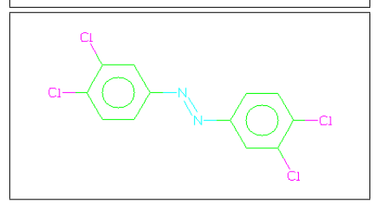
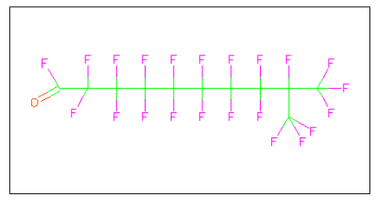
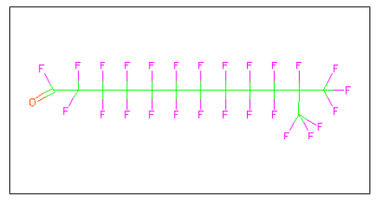
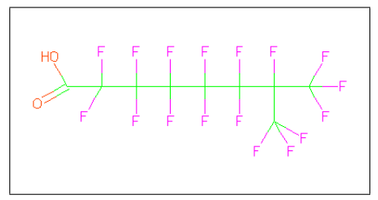
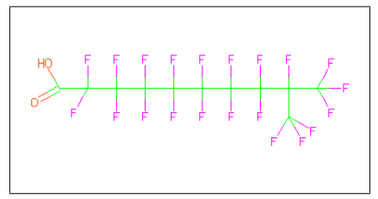
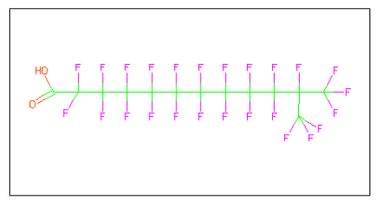
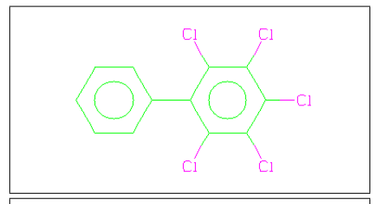
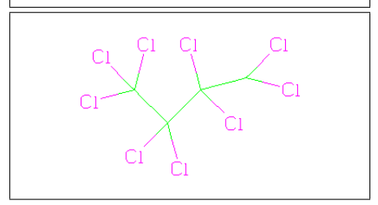
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
37	376-06-7	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.49e+04$	$1.00e+01$	$4.05e+06$	$4.71e-07$	$4.12e-05$	$2.06e+01$	8.83	*Yes*
38	376-22-7	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.11e+03$	$8.17e+03$	$2.89e+06$	*NA*	$1.67e-02$	$1.38e+01$	6.43	*Yes*
39	376-79-4	FC(=C(F)C(F)(Cl)C(F)(Cl)C(F)(Cl)C(F)(Cl)C(F)(Cl)Cl)Cl		$1.09e+03$	$1.29e+04$	$4.90e+06$	$6.06e-06$	$5.80e-04$	$1.38e+01$	7.03	*No*
40	423-50-7	FC(F)(C(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)C(F)(F)C(F)(F)F		$6.41e+02$	$8.99e+03$	$5.32e+05$	$1.91e-03$	$4.80e-02$	$1.00e+06$	6.5	*Yes*
41	423-55-2	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)F		$1.85e+03$	$1.01e+04$	$1.51e+06$	$3.11e-05$	$1.39e-03$	$1.00e+06$	6.57	*Yes*
42	423-62-1	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$7.14e+03$	$2.98e+03$	$2.73e+06$	$1.96e-07$	$1.48e-05$	$1.00e+06$	8.33	*Yes*
43	424-20-4	FC(F)(OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.64e+04$	$1.01e+03$	$1.69e+06$	$4.01e-05$	$3.46e-04$	$1.00e+06$	9.28	*No*
44	507-63-1	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)F		$2.33e+03$	$1.89e+04$	$8.58e+05$	$9.65e-06$	$4.89e-04$	$1.00e+06$	6.99	*Yes*
45	558-96-3	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br)C(F)(F)C(F)(F)C(F)(F)F		$3.24e+03$	$1.01e+04$	$5.20e+06$	$4.48e-06$	$2.45e-04$	$1.00e+06$	7.24	*No*

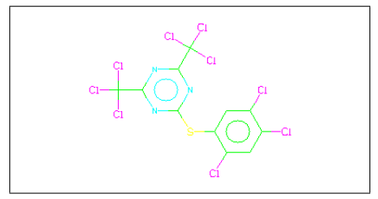
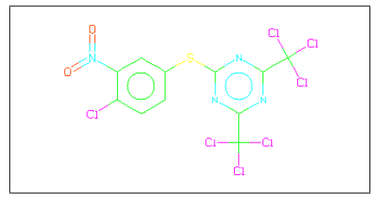
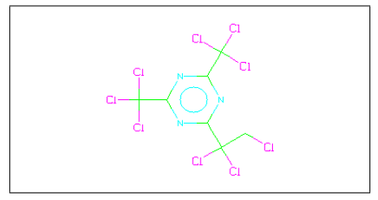
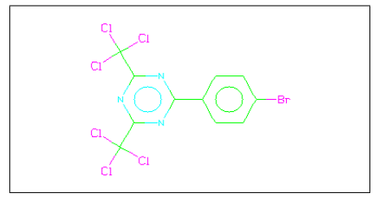
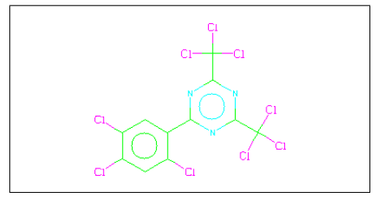
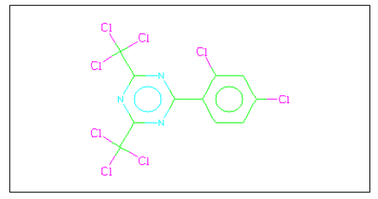
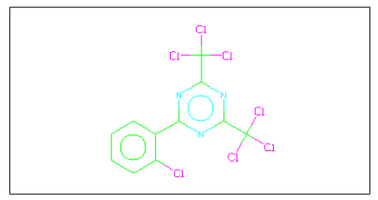
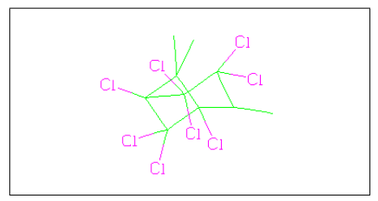
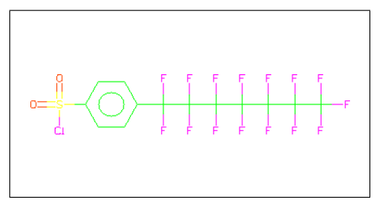
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
46	558-97-4	FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I)C(F)(F)C(F)(F)C(F)(F)F		$4.08e+03$	$6.34e+03$	$2.47e+06$	$1.38e-06$	$8.54e-05$	$1.00e+06$	7.66	*Yes*
47	559-14-8	FC(=C(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)F		$6.36e+02$	$2.96e+03$	$3.84e+05$	$2.89e-04$	$1.00e-02$	$1.38e+01$	5.77	*Yes*
48	677-93-0	FC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$2.11e+04$	$1.14e+03$	$1.30e+06$	$1.58e-08$	$1.53e-06$	$1.00e+06$	9.18	*Yes*
49	737-20-2	Fc1c(F)c(F)c2c(c1F)c(F)c(F)c(c2F)C(Cl)(Cl)Cl		$1.86e+04$	$8.69e+03$	$3.16e+05$	$9.67e-06$	$4.60e-02$	$6.42e+01$	6.47	*No*
50	754-91-6	NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.94e+03$	$3.13e+03$	$6.06e+04$	$1.75e-03$	$6.30e-02$	$1.00e+06$	5.8	*Yes*
51	812-58-8	FC(F)(C(F)(F)Br)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br		$1.32e+03$	$1.86e+04$	$1.35e+06$	$1.03e-05$	$5.19e-04$	$1.00e+06$	6.98	*No*
52	858-46-8	FC(F)(F)C(F)(F)c1nc(nc(n1)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F		$3.17e+03$	$6.86e+02$	$1.38e+05$	$2.70e-02$	$8.00e-03$	$4.13e+01$	5.59	*Yes*
53	865-71-4	FC(F)(F)C(F)(C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F		$1.43e+03$	$1.49e+03$	$5.02e+04$	$9.58e-04$	$3.00e-02$	$1.00e+06$	5.31	*Yes*
54	865-77-0	FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$6.87e+03$	$5.14e+03$	$3.36e+06$	$7.85e-07$	$5.13e-05$	$1.00e+06$	7.84	*Yes*

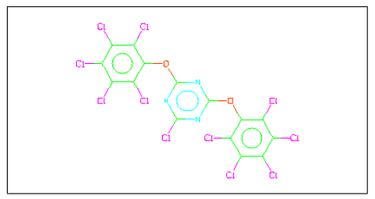
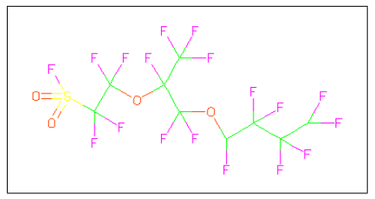
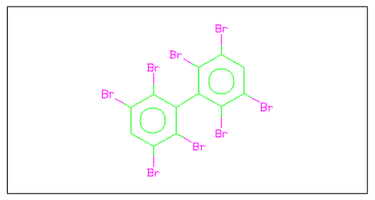
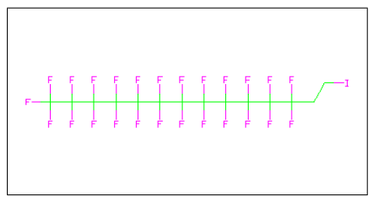
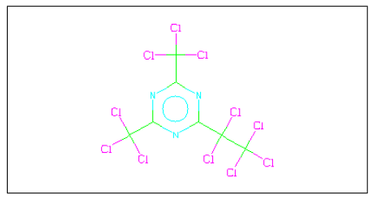
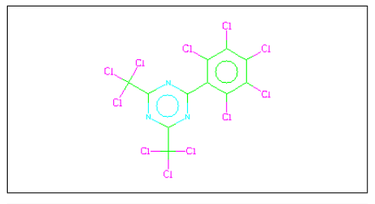
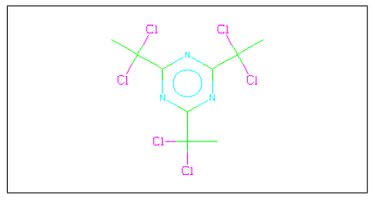
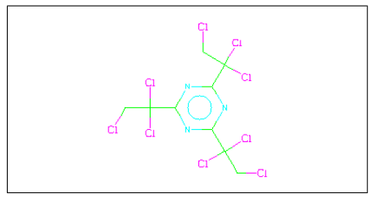
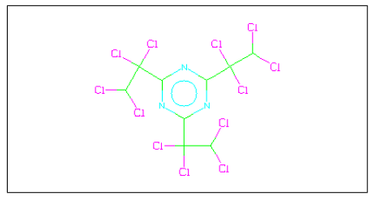
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
55	881-99-2	`ClC(Cl)(Cl)c1cccc(c1)C(Cl)(Cl)Cl`		$3.76e+02$	$3.11e+03$	$1.74e+05$	$3.78e-05$	$6.10e-02$	$1.63e+02$	5.8	*Yes*
56	915-76-4	`FC(F)(C(F)(F)F)C(F)(F)c1nc(nc(n1)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$1.70e+04$	$2.07e+03$	$9.79e+06$	$6.98e-04$	$3.92e-05$	$4.13e+01$	7.59	*Yes*
57	1735-48-4	`FC(F)(F)C(F)(C(F)(C(F)(F)F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F`		$7.38e+03$	$9.63e+03$	$3.89e+06$	$2.99e-05$	$1.33e-03$	$1.00e+06$	6.54	*Yes*
58	1765-48-6	`FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)O`		$1.06e+03$	$5.62e+01$	$1.14e+06$	$1.01e-03$	$4.10e-02$	$2.06e+01$	6.21	*Yes*
59	2043-52-9	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.48e+03$	$9.48e+03$	$7.19e+05$	$3.58e-06$	$1.99e-04$	$1.73e+01$	7.3	*Yes*
60	2043-53-0	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.59e+03$	$4.46e+03$	$1.56e+06$	$5.14e-07$	$3.49e-05$	$1.73e+01$	7.97	*Yes*
61	2043-54-1	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$7.95e+03$	$9.84e+02$	$7.21e+05$	$1.04e-08$	$1.05e-06$	$1.73e+01$	9.31	*Yes*
62	2043-57-4	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.45e+02$	$1.10e+04$	$1.14e+05$	$2.47e-05$	$1.13e-03$	$1.73e+01$	6.63	*Yes*
63	2051-24-3	`Clc1c(Cl)c(Cl)c(Cl)c(c1Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$2.18e+03$	$1.46e+04$	$6.81e+06$	$5.09e-10$	$6.69e-08$	$5.89e+02$	9.235	*Yes*

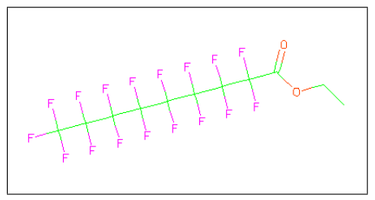
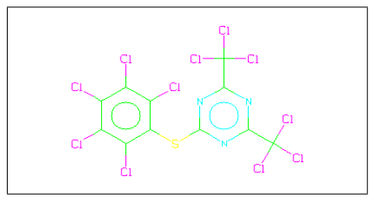
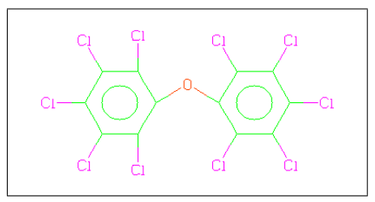
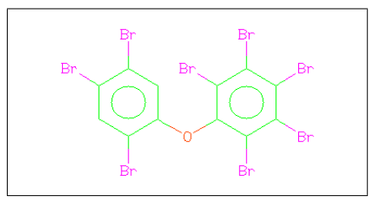
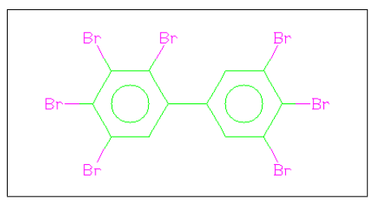
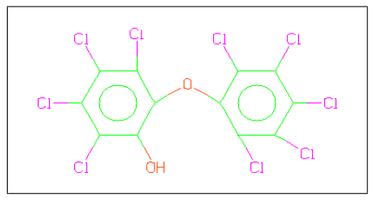
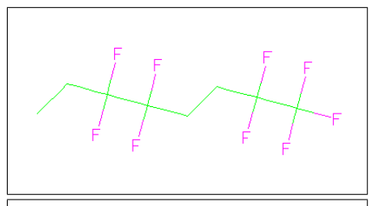
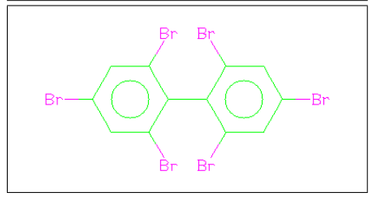
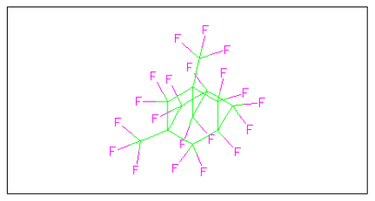
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
64	2058-94-8	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$2.77e+03$	$5.62e+01$	$5.65e+06$	$1.65e-04$	$8.00e-03$	$2.06e+01$	6.82	*Yes*
65	2136-95-0	Clc1c(Cl)c(C(Cl)Cl)c(Cl)c(Cl)c1Cl		$3.51e+02$	$5.70e+03$	$6.25e+04$	$1.63e-05$	$5.20e-02$	$3.37e+01$	6.2	*No*
66	2227-17-0	ClC1=C(Cl)C(Cl)(C(=C1Cl)Cl)C1(Cl)C(=C(Cl)C(=C1Cl)Cl)Cl		$2.33e+03$	$2.77e+03$	$5.69e+06$	$1.19e-07$	$1.86e-05$	$1.36e+01$	8.39	*Yes*
67	2234-13-1	Clc1c(Cl)c(Cl)c(Cl)c2c1c(Cl)c(Cl)c(Cl)c2Cl		$7.40e+02$	$1.89e+03$	$2.22e+05$	$1.23e-07$	$9.27e-06$	$2.78e+02$	8.415	*Yes*
68	3021-63-4	FC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F		$2.26e+04$	$4.93e+03$	$1.07e+07$	$6.32e-07$	$4.17e-05$	$1.00e+06$	7.88	*No*
69	3050-42-8	ClC(=C(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl)Cl		$7.37e+02$	$4.03e+03$	$3.39e+05$	$1.20e-04$	$8.00e-03$	$1.38e+01$	5.97	*No*
70	3268-87-9	Clc1c2Oc3c(Oc2c(Cl)c(Cl)c1Cl)c(Cl)c(Cl)c(Cl)c3Cl		$1.12e+03$	$2.12e+03$	$3.67e+04$	$3.98e-09$	$4.25e-07$	$1.97e+02$	8.85	*No*
71	3330-16-3	FC(OC(F)(F)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)F)C(F)(F)F		$3.22e+04$	$5.24e+03$	$9.86e+06$	$4.45e-04$	$6.00e-03$	$4.13e+03$	7.83	*No*
72	3486-08-6	FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I		$2.24e+03$	$9.09e+03$	$2.85e+05$	$3.79e-05$	$1.67e-03$	$1.00e+06$	6.5	*Yes*

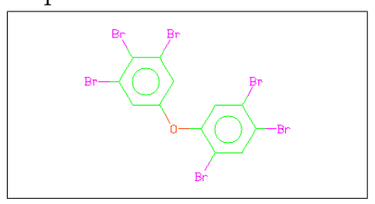
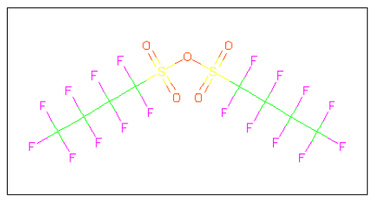
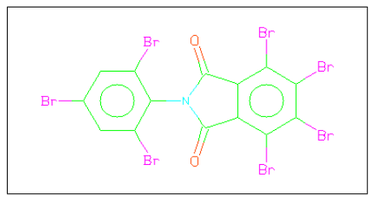
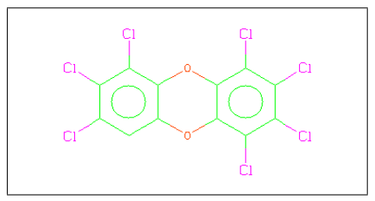
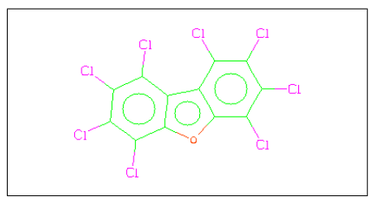
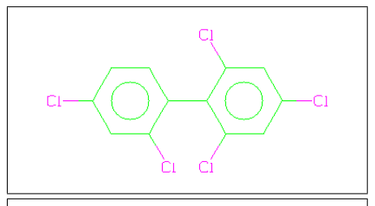
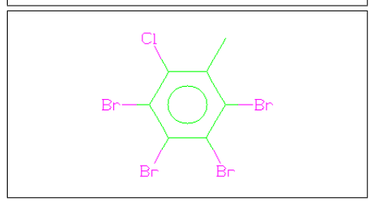
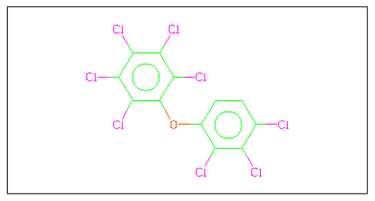
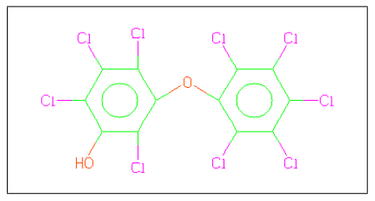
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
73	3658-57-9	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)Cl		$1.30e+03$	$1.00e+01$	$6.42e+05$	$1.79e-03$	$6.70e-02$	$2.06e+01$	5.98	*Yes*
74	3712-60-5	Clc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$1.27e+03$	$1.31e+03$	$4.41e+05$	$3.16e-05$	$2.00e-03$	$1.08e+01$	6.01	*No*
75	3883-86-1	Fc1c(F)cc(F)c(F)c1c1c(F)c(F)cc(F)c1F		$7.99e+03$	$6.16e+03$	$4.40e+04$	$7.36e-04$	$2.30e-02$	$4.52e+01$	5.36	*Yes*
76	4089-58-1	FC(=O)C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F)C(F)(F)F		$2.46e+03$	$2.60e+03$	$5.03e+04$	$8.00e-03$	$2.74e-01$	$1.00e+06$	5.68	*Yes*
77	6820-74-2	ClC(C(Cl)(Cl)Cl)(C(Cl)(Cl)Cl)C(Cl)(Cl)Cl		$3.69e+03$	$9.24e+03$	$1.24e+06$	$2.98e-05$	$1.31e-03$	$1.00e+06$	6.52	*No*
78	6928-57-0	ClC1=C(Cl)C(Cl)(C(=C1Cl)Cl)C(Cl)(Cl)Cl		$8.08e+02$	$5.84e+03$	$5.70e+05$	$6.20e-05$	$4.00e-03$	$2.72e+01$	6.21	*No*
79	7497-08-7	O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl		$2.75e+03$	$6.68e+02$	$5.49e+05$	$6.80e-10$	$8.24e-05$	$1.26e+02$	9.65	*No*
80	7497-11-2	O=C(Oc1c(Cl)cc(Cl)cc1Cl)Oc1c(Cl)cc(Cl)cc1Cl		$3.86e+02$	$1.22e+04$	$3.34e+06$	$1.31e-05$	$7.00e-03$	$1.07e+01$	7.07	*Yes*
81	10386-84-2	Fc1c(Br)c(F)c(F)c(c1F)c1c(F)c(F)c(Br)c(F)c1F		$2.35e+04$	$4.38e+04$	$2.77e+06$	$5.06e-06$	$2.69e-04$	$1.55e+02$	7.14	*Yes*

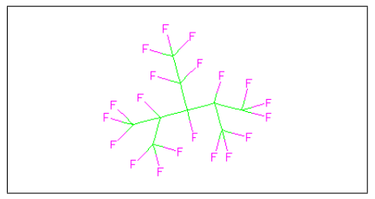
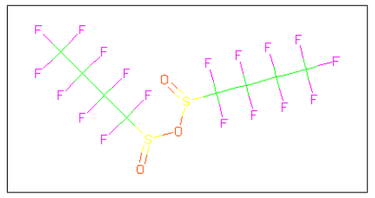
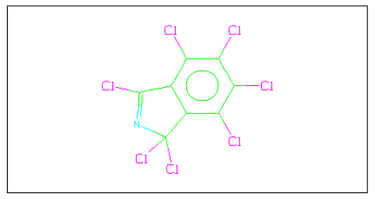
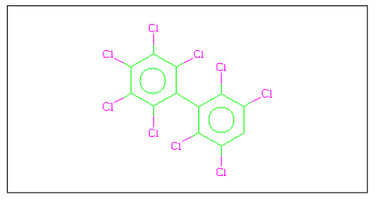
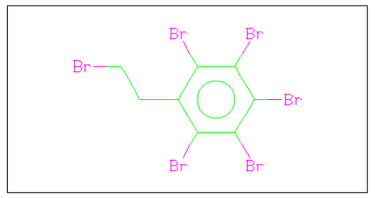
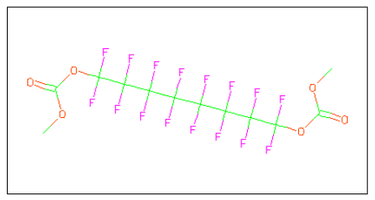
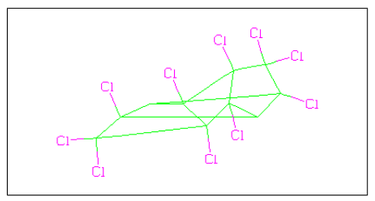
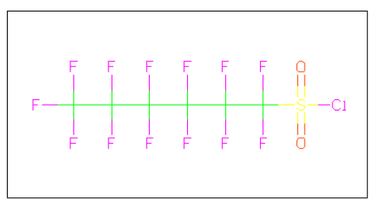
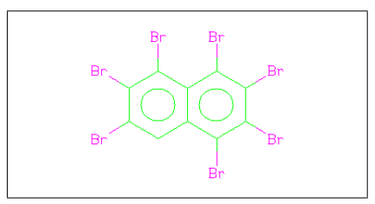
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
82	13075-01-9	`Brc1c(Cl)c(Cl)c(Br)c(Br)c1Cl`		$2.64e+02$	$1.05e+04$	$1.59e+05$	$2.42e-05$	$1.09e-03$	$7.34e+02$	6.6	*No*
83	14047-09-7	`Clc1ccc(N=Nc2ccc(Cl)c(Cl)c2)cc1Cl`		$2.15e+02$	$1.00e+01$	$2.06e+06$	$1.50e-05$	$6.00e-05$	$3.37e+01$	6.69	*No*
84	15720-98-6	`FC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$8.86e+03$	$5.19e+03$	$1.51e+06$	$5.00e-03$	$1.31e-01$	$1.00e+06$	6.14	*Yes*
85	15811-52-6	`FC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$2.72e+04$	$7.80e+03$	$1.10e+07$	$7.68e-04$	$1.20e-02$	$1.00e+06$	7.47	*Yes*
86	15899-31-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.52e+03$	$1.00e+01$	$2.85e+05$	$4.00e-03$	$1.54e-01$	$2.06e+01$	5.67	*Yes*
87	16486-94-5	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$4.67e+03$	$5.62e+01$	$7.81e+06$	$9.37e-05$	$5.00e-03$	$2.06e+01$	7.01	*Yes*
88	16486-96-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.43e+04$	$1.00e+01$	$7.82e+06$	$1.90e-06$	$1.44e-04$	$2.06e+01$	8.35	*Yes*
89	18259-05-7	`Clc1c(c2ccccc2)c(Cl)c(Cl)c(Cl)c1Cl`		$1.80e+02$	$6.00e+04$	$1.33e+06$	$5.91e-06$	$2.99e-04$	$1.55e+01$	6.865	*No*
90	21483-62-5	`ClC(Cl)C(Cl)(Cl)C(Cl)(Cl)C(Cl)(Cl)Cl`		$1.66e+03$	$6.66e+03$	$4.07e+05$	$5.25e-05$	$2.00e-03$	$1.53e+02$	6.3	*No*

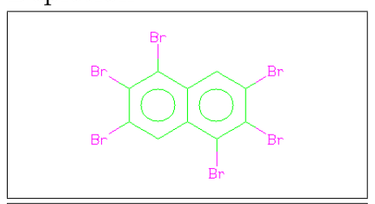
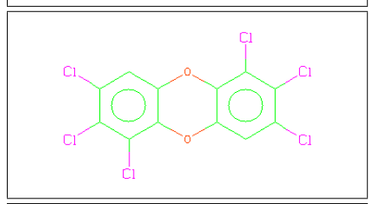
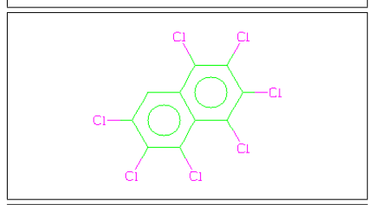
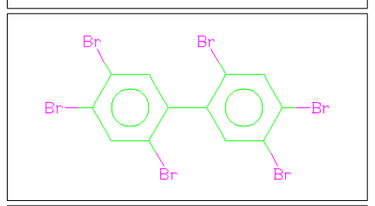
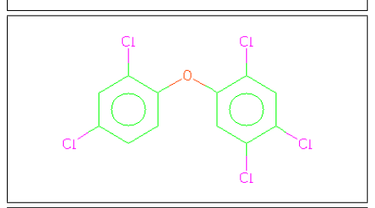
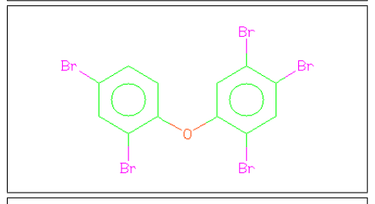
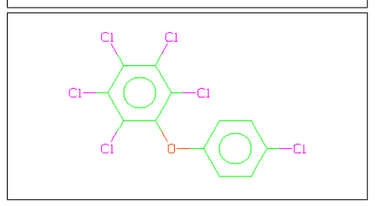
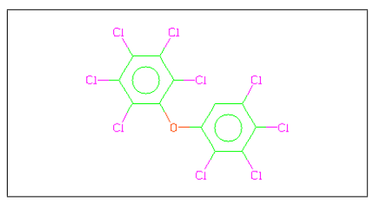
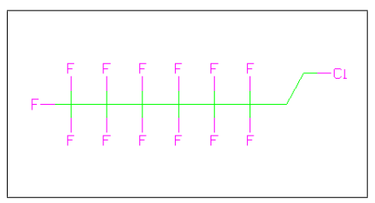
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{OW}$	PR
91	24478-11-3	`Clc1cc(Cl)c(Cl)cc1Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.85e+03$	$1.58e+03$	$5.11e+06$	$6.22e-07$	$1.79e-05$	$1.41e+01$	7.84	*No*
92	24478-15-7	`O=N(=O)c1cc(ccc1Cl)Sc1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.30e+03$	$2.24e+03$	$1.90e+05$	$1.68e-05$	$1.05e-03$	$3.30e+01$	6.36	*No*
93	24481-33-2	`ClCC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.44e+03$	$1.28e+03$	$1.65e+05$	$3.43e-05$	$3.00e-03$	$1.13e+02$	6	*No*
94	24481-49-0	`Brc1ccc(cc1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.34e+03$	$1.90e+03$	$6.58e+05$	$2.00e-05$	$1.33e-03$	$1.10e+01$	6.26	*No*
95	24481-50-3	`Clc1cc(Cl)c(Cl)cc1c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$3.40e+03$	$2.35e+03$	$1.41e+06$	$1.54e-05$	$9.50e-04$	$5.23e+01$	6.4	*No*
96	24481-52-5	`Clc1ccc(c(Cl)c1)c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$2.08e+03$	$8.82e+02$	$2.07e+05$	$6.20e-05$	$5.00e-03$	$1.55e+01$	5.75	*No*
97	24481-55-8	`Clc1ccccc1c1nc(nc(n1)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.27e+03$	$3.31e+02$	$2.02e+04$	$2.48e-04$	$3.00e-02$	$1.08e+01$	5.11	*No*
98	25267-15-6	`CC1C(Cl)(Cl)C(Cl)(Cl)C2(Cl)C(C)(C)C1(Cl)C2(Cl)Cl`		$4.41e+03$	$3.88e+03$	$4.51e+06$	$2.56e-07$	$1.80e-05$	$1.08e+01$	8.09	*No*
99	25444-35-3	`ClS(=O)(=O)c1ccc(cc1)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$1.60e+03$	$3.37e+03$	$3.93e+06$	$2.14e-04$	$2.00e-03$	$1.16e+01$	8.22	*Yes*

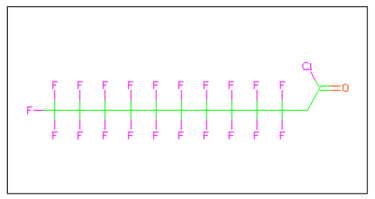
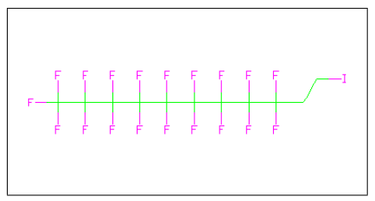
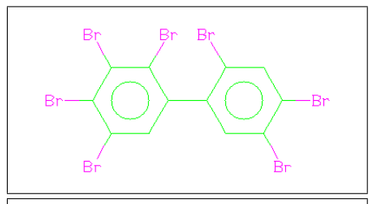
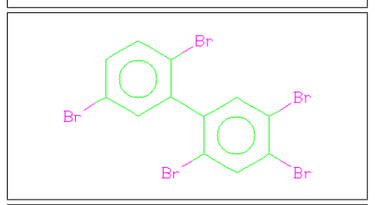
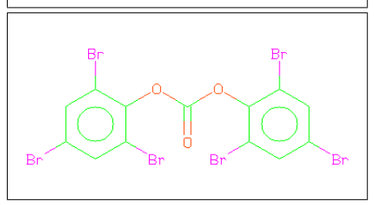
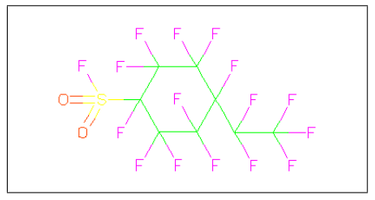
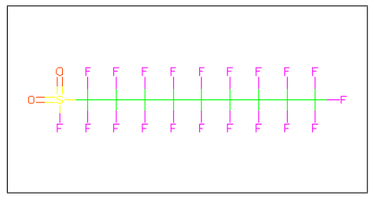
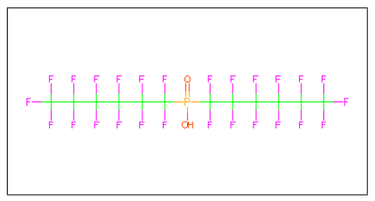
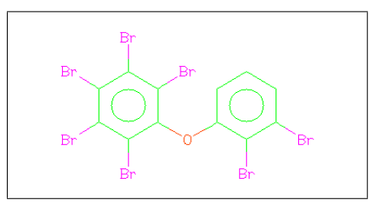
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
100	26396-34-9	`Clc1nc(nc(n1)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$1.03e+04$	$2.95e+02$	$1.02e+06$	$2.55e-05$	$3.40e-07$	$1.07e+02$	9.32	*No*
101	26654-97-7	`FC(OC(F)(F)C(F)(OC(F)(F)C(F)(F)S(=O)(=O)F)C(F)(F)F)C(F)(F)C(F)(F)C(F)F`		$1.67e+03$	$6.34e+03$	$2.57e+06$	$4.84e-04$	$7.00e-03$	$1.10e+04$	7.66	*No*
102	27858-07-7	`Brc1c(Br)cc(Br)c(Br)c1c1c(Br)c(Br)cc(Br)c1Br`		$1.20e+03$	$7.62e+03$	$2.47e+04$	$1.03e-10$	$1.66e-08$	$2.48e+02$	8.19	*Yes*
103	30046-31-2	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.44e+04$	$2.18e+02$	$7.33e+04$	$2.05e-10$	$3.08e-08$	$1.73e+01$	10.65	*Yes*
104	30362-35-7	`ClC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl`		$1.18e+04$	$3.61e+03$	$3.79e+06$	$3.24e-06$	$1.38e-04$	$1.77e+03$	7.1	*No*
105	30362-55-1	`Clc1c(c2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$9.10e+03$	$1.87e+03$	$6.48e+06$	$9.37e-07$	$2.92e-05$	$2.52e+02$	7.69	*No*
106	30362-74-4	`CC(Cl)(Cl)c1nc(nc(n1)C(C)(Cl)Cl)C(C)(Cl)Cl`		$1.04e+03$	$1.79e+03$	$1.53e+05$	$1.73e-05$	$1.17e-03$	$2.96e+01$	6.22	*No*
107	30362-75-5	`ClCC(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl`		$3.83e+03$	$5.71e+03$	$1.64e+06$	$3.91e-06$	$1.77e-04$	$2.04e+01$	6.98	*No*
108	30362-76-6	`ClC(Cl)C(Cl)(Cl)c1nc(nc(n1)C(Cl)(Cl)C(Cl)Cl)C(Cl)(Cl)C(Cl)Cl`		$1.40e+04$	$2.24e+03$	$4.28e+06$	$1.39e-06$	$4.73e-05$	$2.28e+01$	7.52	*No*

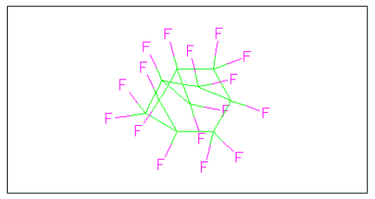
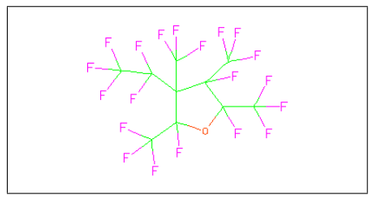
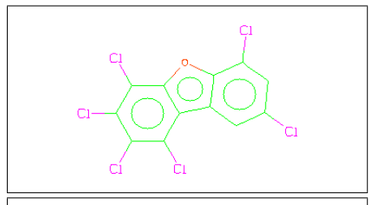
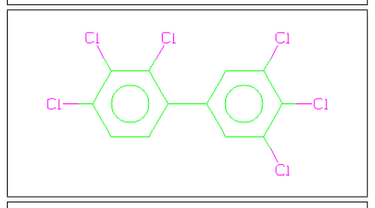
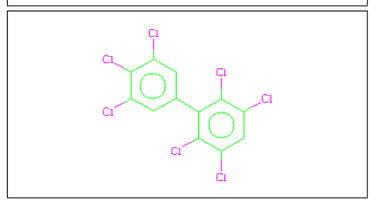
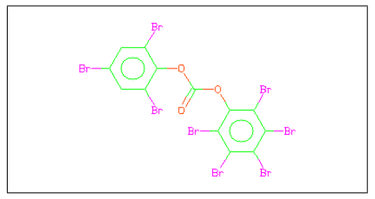
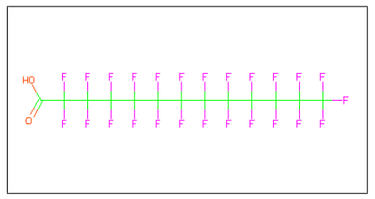
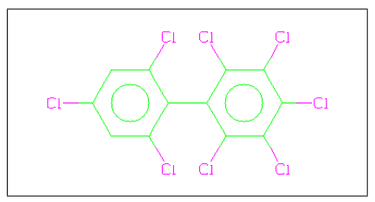
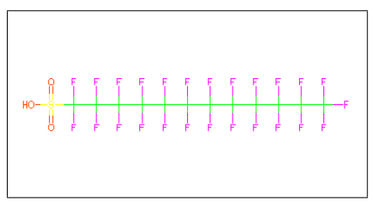
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
109	30377-52-7	CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$1.48e+03$	$6.28e+03$	$2.62e+04$	$1.47e-03$	$4.60e-02$	$1.17e+01$	6.26	*Yes*
110	31007-95-1	Clc1c(Sc2nc(nc(n2)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl)c(Cl)c(Cl)c(Cl)c1Cl		$1.03e+04$	$3.68e+02$	$1.42e+06$	$3.76e-08$	$5.47e-07$	$6.77e+01$	9.13	*No*
111	31710-30-2	Clc1c(Cl)c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl		$2.57e+03$	$3.59e+03$	$8.42e+05$	$2.77e-09$	$3.09e-07$	$2.19e+02$	8.905	*No*
112	32536-52-0	Brc1cc(Br)c(Br)cc1Oc1c(Br)c(Br)c(Br)c(Br)c1Br		$1.41e+03$	$1.93e+03$	$3.95e+05$	$5.55e-10$	$7.58e-08$	$9.36e+01$	9.52	*Yes*
113	35194-78-6	Brc1c(Br)cc(cc1Br)c1cc(Br)c(Br)c(Br)c1Br		$7.00e+02$	$1.76e+03$	$2.15e+05$	$1.38e-09$	$1.71e-07$	$9.77e+01$	9.99	*No*
114	35245-80-8	Oc1c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1Cl		$1.52e+03$	$2.37e+03$	$4.69e+05$	$9.36e-05$	$1.71e-05$	$1.41e+01$	8.53	*No*
115	35262-54-5	CCC(F)(F)C(F)(F)CCC(F)(F)C(F)(F)F		$1.89e+02$	$5.00e+03$	$9.52e+04$	$6.98e-05$	$3.00e-03$	$4.74e+01$	6.11	*No*
116	36355-01-8	Brc1cc(Br)c(c(Br)c1)c1c(Br)cc(Br)cc1Br		$4.08e+02$	$3.68e+04$	$4.14e+06$	$1.83e-08$	$1.74e-06$	$3.78e+01$	7.745	*Yes*
117	36481-20-6	FC12C(F)(F)C3(C(F)(F)F)C(F)(F)C(C(F)(F)F)(C1(F)F)C(F)(F)C(F)(C3(F)F)C2(F)F		$1.58e+04$	$2.96e+03$	$3.96e+06$	$1.56e-07$	$1.18e-05$	$1.00e+06$	8.33	*No*

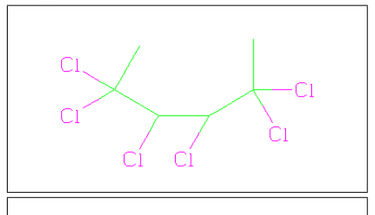
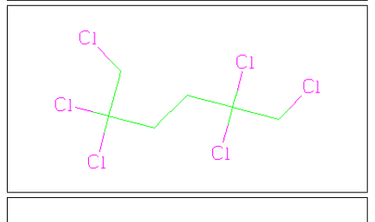
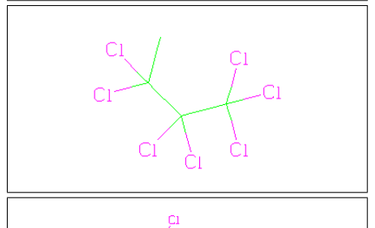
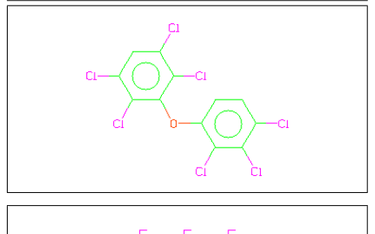
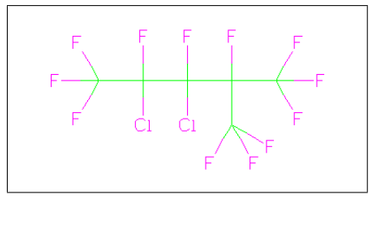
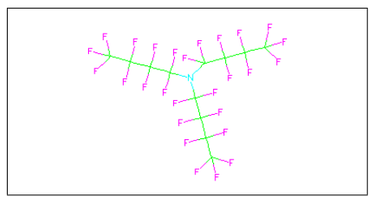
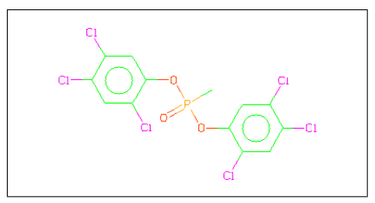
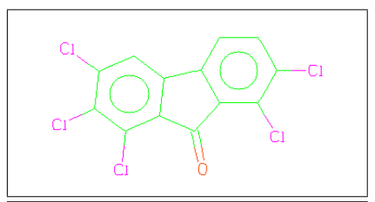
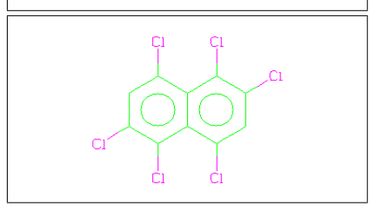
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
118	36483-60-0	`Brc1cc(Br)c(Br)cc1Oc1cc(Br)c(Br)c(Br)c1`		$4.81e+02$	$2.91e+03$	$8.13e+05$	$9.91e-08$	$7.98e-06$	$3.04e+01$	7.975	*Yes*
119	36913-91-4	`FC(F)(S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F`		$4.51e+03$	$3.17e+03$	$3.13e+06$	$2.08e-07$	$1.55e-05$	$1.00e+06$	8.27	*Yes*
120	37710-57-9	`Brc1cc(Br)c(c(Br)c1)N1C(=O)c2c(C1=O)c(Br)c(Br)c(Br)c2Br`		$9.13e+02$	$4.77e+03$	$1.43e+06$	$1.21e-04$	$2.00e-03$	$3.84e+01$	7.91	*No*
121	37871-00-4	`Clc1c(Cl)cc2Oc3c(Oc2c1Cl)c(Cl)c(Cl)c(Cl)c3Cl`		$6.87e+02$	$4.47e+03$	$6.69e+04$	$2.61e-08$	$2.30e-06$	$7.72e+01$	8.425	*No*
122	39001-02-0	`Clc1c(Cl)c2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl`		$8.63e+02$	$1.30e+03$	$2.41e+04$	$2.58e-08$	$2.28e-06$	$1.00e+03$	8.735	*No*
123	39485-83-1	`Clc1ccc(c(Cl)c1)c1c(Cl)cc(Cl)cc1Cl`		$1.87e+02$	$7.21e+04$	$6.76e+06$	$5.91e-06$	$2.99e-04$	$1.89e+01$	6.98	*No*
124	39569-21-6	`Clc1c(C)c(Br)c(Br)c(Br)c1Br`		$2.04e+02$	$1.12e+04$	$3.99e+04$	$1.63e-05$	$7.70e-04$	$5.61e+01$	6.74	*Yes*
125	40356-57-8	`Clc1ccc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1Cl`		$9.62e+02$	$5.16e+03$	$5.54e+06$	$1.20e-07$	$9.15e-06$	$7.18e+01$	8.105	*No*
126	42255-14-1	`Clc1c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1O`		$1.52e+03$	$2.37e+03$	$4.69e+05$	$9.36e-05$	$1.71e-05$	$1.72e+01$	8.53	*No*

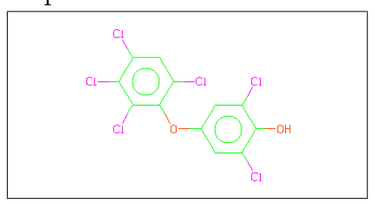
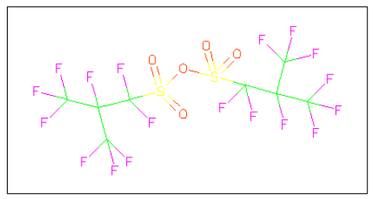
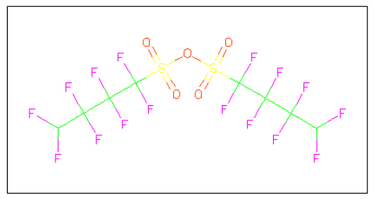
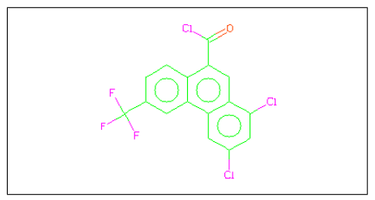
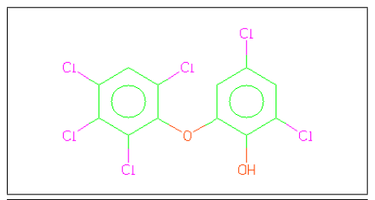
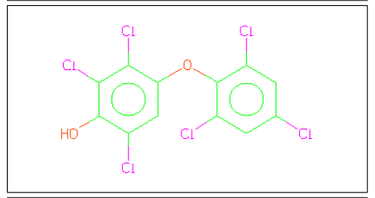
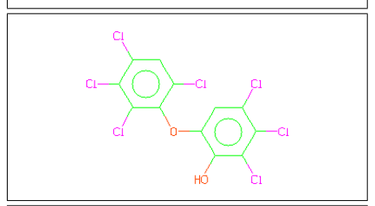
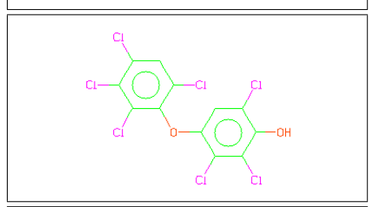
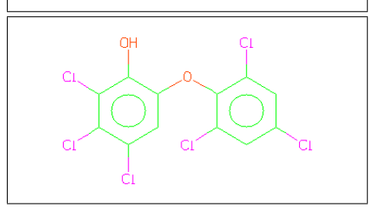
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
127	50285-18-2	FC(F)(C(F)(F)F)C(F)(C(F)(C(F)(F)F)C(F)(F)F)C(F)(C(F)(F)F)C(F)(F)F		$2.18e+04$	$1.43e+04$	$7.28e+06$	$1.51e-05$	$7.23e-04$	$1.00e+06$	6.8	*Yes*
128	51735-74-1	O=S(OS(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$3.99e+03$	$4.70e+03$	$4.50e+06$	$5.70e-07$	$3.81e-05$	$1.00e+06$	7.92	*No*
129	52135-26-9	Clc1c(Cl)c2C(=NC(Cl)(Cl)c2c(Cl)c1Cl)Cl		$5.27e+02$	$8.05e+03$	$4.95e+06$	$1.03e-06$	$7.00e-03$	$4.92e+01$	7.45	*No*
130	52663-77-1	Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)c1c(Cl)c(Cl)cc(Cl)c1Cl		$1.34e+03$	$1.38e+04$	$6.10e+06$	$3.35e-09$	$3.64e-07$	$3.25e+02$	8.86	*No*
131	53097-60-2	BrCCc1c(Br)c(Br)c(Br)c(Br)c1Br		$2.90e+02$	$5.25e+03$	$3.92e+04$	$8.05e-07$	$5.23e-05$	$1.34e+01$	7.82	*Yes*
132	55521-14-7	COC(=O)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(=O)OC		$1.40e+03$	$5.64e+03$	$1.88e+05$	$5.55e-04$	$4.80e-02$	$2.46e+01$	6.19	*No*
133	55570-84-8	ClC12C3C4(Cl)C(Cl)(C2(Cl)Cl)C2(Cl)C1C3(Cl)C(Cl)(Cl)C42Cl		$2.14e+04$	$1.71e+04$	$3.77e+06$	$2.92e-05$	$1.31e-03$	$1.40e+01$	6.92	*No*
134	55591-23-6	FC(F)(C(F)(F)C(F)(F)S(=O)(=O)Cl)C(F)(F)C(F)(F)C(F)(F)F		$6.83e+02$	$1.45e+04$	$2.77e+05$	*NA*	$6.48e-03$	$1.00e+06$	6.81	*Yes*
135	55688-01-2	Brc1cc2c(c(Br)c1Br)c(Br)c(Br)c(Br)c2Br		$6.34e+02$	$3.42e+03$	$1.12e+05$	$7.95e-09$	$8.24e-07$	$1.98e+02$	9.4	*No*

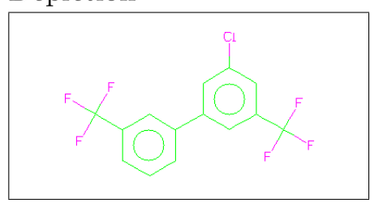
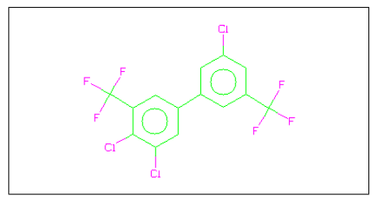
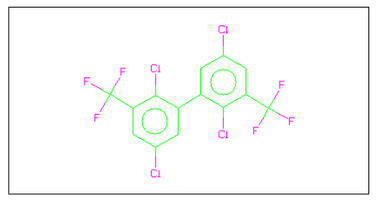
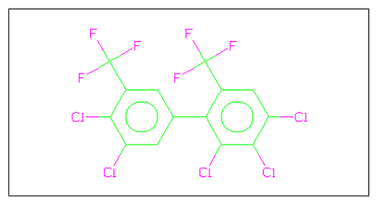
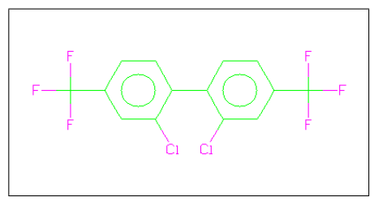
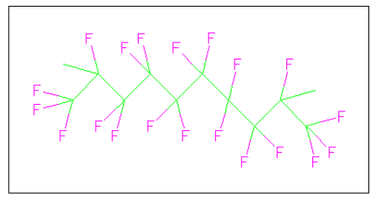
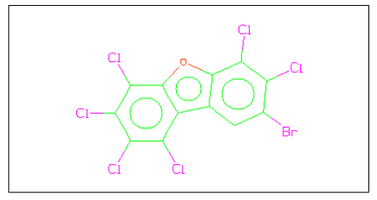
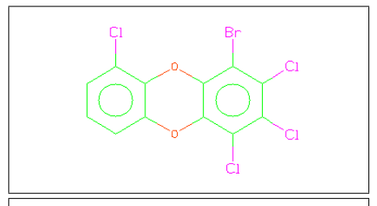
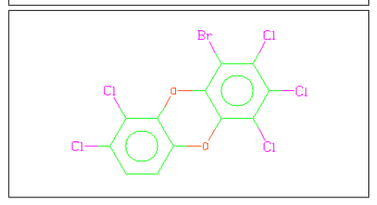
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
136	56480-06-9	`Brc1c(Br)cc2c(Br)c(Br)c(Br)cc2c1Br`		$3.70e+02$	$9.34e+03$	$3.38e+05$	$1.05e-07$	$8.34e-06$	$8.43e+01$	8.51	*Yes*
137	57653-85-7	`Clc1cc2Oc3c(cc(Cl)c(Cl)c3Cl)Oc2c(Cl)c1Cl`		$4.21e+02$	$5.36e+03$	$4.79e+04$	$1.69e-07$	$1.23e-05$	$3.41e+01$	8.21	*No*
138	58863-14-2	`Clc1cc2c(c(Cl)c1Cl)c(Cl)c(Cl)c(Cl)c2Cl`		$4.53e+02$	$1.32e+04$	$2.85e+06$	$7.95e-07$	$4.95e-05$	$1.26e+02$	7.94	*No*
139	59080-40-9	`Brc1cc(Br)c(Br)cc1c1cc(Br)c(Br)cc1Br`		$4.08e+02$	$4.81e+03$	$1.13e+06$	$1.83e-08$	$1.74e-06$	$8.30e+01$	9.1	*No*
140	60123-64-0	`Clc1ccc(Oc2cc(Cl)c(Cl)cc2Cl)c(Cl)c1`		$2.20e+02$	$1.10e+04$	$1.63e+06$	$3.26e-05$	$1.40e-03$	$1.56e+01$	6.405	*No*
141	60348-60-9	`Brc1ccc(Oc2cc(Br)c(Br)cc2Br)c(Br)c1`		$2.80e+02$	$1.51e+04$	$2.36e+06$	$1.30e-06$	$8.02e-05$	$1.94e+01$	7.25	*No*
142	63646-56-0	`Clc1ccc(cc1)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl`		$3.60e+02$	$1.79e+04$	$3.19e+06$	$5.08e-06$	$2.64e-04$	$1.71e+01$	7.015	*No*
143	63919-04-0	`Clc1cc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl`		$1.57e+03$	$3.98e+03$	$5.25e+06$	$1.83e-08$	$1.69e-06$	$1.21e+02$	8.54	*No*
144	64018-25-3	`ClCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$8.03e+02$	$5.12e+03$	$3.83e+05$	*NA*	$2.84e-02$	$2.42e+01$	6.13	*Yes*

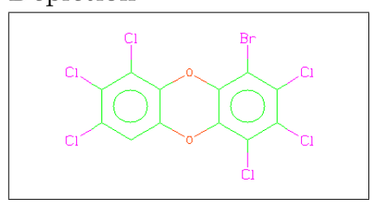
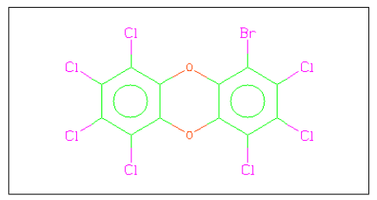
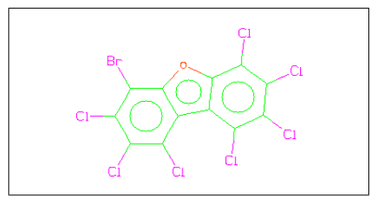
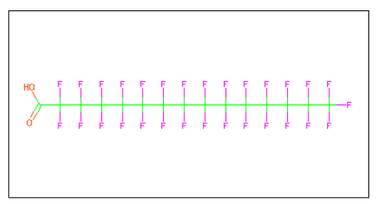
Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
145	64018-26-4	`ClC(=O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$5.91e+03$	$1.33e+04$	$2.19e+06$	NA	$1.06e-02$	$9.47e+03$	6.75	*Yes*
146	65510-56-7	`ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$4.54e+03$	$2.10e+03$	$1.41e+06$	$7.33e-08$	$6.07e-06$	$1.73e+01$	8.64	*Yes*
147	67733-52-2	`Brc1cc(Br)c(Br)cc1c1cc(Br)c(Br)c(Br)c1Br`		$7.00e+02$	$1.76e+03$	$2.15e+05$	$1.38e-09$	$1.71e-07$	$1.31e+02$	9.99	*No*
148	67888-96-4	`Brc1ccc(Br)c(c1)c1cc(Br)c(Br)cc1Br`		$2.38e+02$	$4.58e+04$	$3.25e+06$	$2.39e-07$	$1.74e-05$	$3.78e+01$	7.655	*No*
149	67990-32-3	`O=C(Oc1c(Br)cc(Br)cc1Br)Oc1c(Br)cc(Br)cc1Br`		$5.14e+02$	$2.32e+03$	$6.53e+05$	$6.48e-08$	$7.77e-04$	$1.50e+01$	8.55	*Yes*
150	68156-06-9	`FC1(S(=O)(=O)F)C(F)(F)C(F)(F)C(F)(C(F)(F)C1(F)F)C(F)(F)C(F)(F)F`		$1.70e+03$	$5.65e+03$	$1.35e+06$	$3.53e-04$	$5.00e-03$	$1.00e+06$	7.76	*Yes*
151	68259-06-3	`FC(F)(C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)S(=O)(=O)F`		$3.44e+03$	$2.44e+03$	$3.66e+06$	$1.43e-04$	$1.33e-03$	$1.00e+06$	8.5	*Yes*
152	68412-69-1	`FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)P(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$3.12e+04$	$1.82e+04$	$7.82e+06$	$1.34e-05$	$6.76e-04$	$7.64e+01$	6.96	*Yes*
153	68928-80-3	`Brc1cccc(Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c1Br`		$8.24e+02$	$8.48e+02$	$2.17e+05$	$7.46e-09$	$7.83e-07$	$3.55e+01$	9.44	*Yes*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
154	69064-33-1	FC12C(F)(F)C3(F)C(F)(F)C(F)(C1(F)F)C(F)(F)C(F)(C2(F)F)C3(F)F		$1.81e+03$	$7.75e+03$	$2.07e+05$	$4.46e-05$	$1.90e-03$	$1.00e+06$	6.4	*No*
155	69661-30-9	FC(F)(F)C1(C(F)(F)C(F)(F)F)C(F)(OC(F)(C(F)(F)F)C1(F)C(F)(F)F)C(F)(F)F		$3.56e+04$	$1.03e+04$	$7.15e+06$	*NA*	$3.11e-03$	$1.00e+06$	7.22	*Yes*
156	69698-60-8	Clc1cc(Cl)c2oc3c(Cl)c(Cl)c(Cl)c(Cl)c3c2c1		$3.23e+02$	$6.90e+03$	$6.47e+04$	$1.09e-06$	$6.59e-05$	$2.06e+02$	7.58	*No*
157	69782-90-7	Clc1ccc(c2cc(Cl)c(Cl)c(Cl)c2)c(Cl)c1Cl		$3.06e+02$	$2.61e+04$	$9.38e+06$	$9.23e-07$	$5.65e-05$	$4.57e+01$	7.61	*No*
158	69782-91-8	Clc1c(Cl)cc(cc1Cl)c1c(Cl)c(Cl)cc(Cl)c1Cl		$5.01e+02$	$1.23e+04$	$7.04e+06$	$1.43e-07$	$1.06e-05$	$7.64e+01$	8.27	*No*
159	71216-04-1	Brc1cc(Br)c(OC(=O)Oc2c(Br)c(Br)c(Br)c(Br)c2Br)c(Br)c1		$1.51e+03$	$3.12e+02$	$4.38e+04$	$7.22e-11$	$3.59e-05$	$2.77e+01$	10.33	*No*
160	72629-94-8	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		$8.49e+03$	$1.00e+01$	$8.83e+06$	$3.34e-06$	$2.40e-04$	$2.06e+01$	8.16	*Yes*
161	74472-52-9	Clc1cc(Cl)c(c(Cl)c1)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl		$8.18e+02$	$5.92e+03$	$3.03e+06$	$2.20e-08$	$1.97e-06$	$8.67e+01$	8.91	*No*
162	79780-39-5	FC(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)O		$1.31e+04$	$5.62e+01$	$5.87e+06$	*NA*	$4.73e-03$	$7.64e+01$	7.17	*Yes*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
163	83682-28-4	`ClC(C(Cl)C(C)(Cl)Cl)C(C)(Cl)Cl`		$3.48e+02$	$3.38e+03$	$2.78e+04$	$1.62e-04$	$6.00e-03$	$5.33e+01$	5.85	*No*
164	83682-29-5	`ClCC(Cl)(Cl)CCC(Cl)(Cl)CCl`		$3.48e+02$	$4.22e+03$	$4.23e+04$	$1.04e-04$	$4.00e-03$	$1.42e+01$	6	*No*
165	83682-70-6	`ClC(Cl)(C(C)(Cl)Cl)C(Cl)(Cl)Cl`		$6.96e+02$	$3.44e+03$	$6.70e+04$	$1.60e-04$	$6.00e-03$	$3.15e+02$	5.86	*No*
166	83992-71-6	`Clc1ccc(Oc2c(Cl)c(Cl)cc(Cl)c2Cl)c(Cl)c1Cl`		$5.89e+02$	$1.14e+04$	$4.17e+06$	$7.83e-07$	$4.94e-05$	$5.19e+01$	7.43	*No*
167	85720-79-2	`FC(Cl)(C(F)(F)F)C(F)(Cl)C(F)(C(F)(F)F)C(F)(F)F`		$2.95e+03$	$3.86e+03$	$5.33e+05$	*NA*	$4.26e-02$	$1.00e+06$	5.94	*Yes*
168	311-89-7	`FC(F)(N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F`		$1.46e+05$	$3.44e+03$	$6.16e+06$	$2.43e-04$	$3.00e-03$	$1.00e+06$	8.2	*Yes*
169	88847-67-0	`Clc1cc(Cl)c(Cl)cc1OP(=O)(C)Oc1cc(Cl)c(Cl)cc1Cl`		$4.39e+02$	$1.46e+04$	$3.42e+06$	$3.90e-05$	$1.20e-02$	$1.88e+01$	6.82	*No*
170	90077-77-3	`Clc1ccc2c(c1Cl)C(=O)c1c2cc(Cl)c(Cl)c1Cl`		$2.15e+02$	$3.56e+03$	$3.34e+04$	$1.19e-05$	$5.68e-04$	$2.48e+01$	6.77	*No*
171	90948-28-0	`Clc1cc(Cl)c2c(Cl)c(Cl)cc(Cl)c2c1Cl`		$2.77e+02$	$4.92e+04$	$1.92e+06$	$5.10e-06$	$2.63e-04$	$5.72e+01$	7.04	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	log K_{OW}	PR
172	90986-11-1	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.36e+01$	6.6	*No*
173	93894-52-1	`FC(F)(F)C(F)(C(F)(F)F)C(F)(F)S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F`		$1.28e+04$	$4.07e+03$	$5.44e+06$	*NA*	$5.19e-04$	$1.00e+06$	8.05	*Yes*
174	93894-55-4	`FC(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)F`		$6.61e+02$	$1.25e+04$	$4.60e+05$	*NA*	$4.76e-03$	$1.73e+04$	7.06	*Yes*
175	94133-67-2	`Clc1cc(Cl)c2cc(C(=O)Cl)c3ccc(cc3c2c1)C(F)(F)F`		$1.89e+02$	$2.06e+04$	$2.44e+03$	*NA*	$3.44e-02$	$3.71e+01$	6.04	*Yes*
176	94888-10-5	`Clc1cc(Oc2c(Cl)cc(Cl)c(Cl)c2Cl)c(O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.36e+01$	6.6	*No*
177	94888-11-6	`Clc1cc(Cl)c(Oc2cc(Cl)c(O)c(Cl)c2Cl)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.53e+01$	6.6	*No*
178	94888-12-7	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(Cl)c(Cl)c1O`		$5.68e+02$	$1.01e+04$	$2.92e+05$	$1.02e-03$	$2.83e-04$	$2.71e+01$	7.24	*No*
179	94888-13-8	`Clc1cc(Cl)c(Cl)c(Cl)c1Oc1cc(Cl)c(O)c(Cl)c1Cl`		$5.68e+02$	$1.01e+04$	$2.92e+05$	$1.02e-03$	$2.83e-04$	$2.71e+01$	7.24	*No*
180	94897-81-1	`Clc1cc(Cl)c(Oc2cc(Cl)c(Cl)c(Cl)c2O)c(Cl)c1`		$3.47e+02$	$1.05e+04$	$6.90e+04$	$3.00e-03$	$1.14e-03$	$1.53e+01$	6.6	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
181	95998-64-4	`Clc1cc(cc(c1)C(F)(F)F)c1cccc(c1)C(F)(F)F`		$2.63e+02$	$6.95e+03$	$3.44e+06$	$4.25e-05$	$1.77e-03$	$1.45e+01$	6.33	*No*
182	95998-66-6	`Clc1cc(cc(c1)C(F)(F)F)c1cc(Cl)c(Cl)c(c1)C(F)(F)F`		$7.03e+02$	$6.64e+03$	$1.17e+07$	$1.03e-06$	$6.29e-05$	$4.01e+01$	7.62	*No*
183	95998-67-7	`Clc1cc(c2cc(Cl)cc(c2Cl)C(F)(F)F)c(Cl)c(c1)C(F)(F)F`		$1.15e+03$	$3.21e+03$	$8.56e+06$	$1.58e-07$	$1.17e-05$	$9.68e+01$	8.26	*No*
184	95998-68-8	`Clc1cc(c(c2cc(Cl)c(Cl)c(c2)C(F)(F)F)c(Cl)c1Cl)C(F)(F)F`		$1.88e+03$	$1.55e+03$	$3.59e+06$	$2.42e-08$	$2.16e-06$	$2.11e+02$	8.91	*No*
185	99686-52-9	`Clc1cc(ccc1c1ccc(cc1Cl)C(F)(F)F)C(F)(F)F`		$4.30e+02$	$1.85e+04$	$8.95e+06$	$6.65e-06$	$3.36e-04$	$3.65e+01$	6.97	*No*
186	103188-55-2	`FC(F)(C(F)(F)C(F)(F)C(F)(F)C(C)(F)C(F)(F)F)C(F)(F)C(F)(F)C(C)(F)C(F)(F)F`		$7.72e+03$	$2.78e+03$	$6.18e+06$	$1.34e-07$	$1.03e-05$	$3.93e+01$	8.39	*No*
187	107207-47-6	`Brc1cc2c(oc3c(Cl)c(Cl)c(Cl)c(Cl)c23)c(Cl)c1Cl`		$5.54e+02$	$2.53e+03$	$5.35e+04$	$8.85e-08$	$6.97e-06$	$4.84e+02$	8.47	*No*
188	109264-61-1	`Clc1cccc2Oc3c(Oc12)c(Br)c(Cl)c(Cl)c3Cl`		$2.70e+02$	$5.34e+03$	$1.05e+05$	$5.83e-07$	$3.78e-05$	$1.87e+01$	7.81	*No*
189	109264-65-5	`Clc1ccc2Oc3c(Oc2c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$4.41e+02$	$2.58e+03$	$1.19e+05$	$8.96e-08$	$7.02e-06$	$5.15e+01$	8.45	*No*

Nr	CAS	SMILES	Depiction	Half-life biodeg. [days]	BCF	BAF	NOEC/ChV [mg/L]	LC50/EC50 [mg/L]	Half-life air OH [days]	$\log K_{\mathrm{OW}}$	PR
190	109264-67-7	`Clc1c(Cl)cc2Oc3c(Oc2c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$7.21e+02$	$1.25e+03$	$8.66e+04$	$1.37e-08$	$1.30e-06$	$7.77e+01$	9.1	*No*
191	109264-69-9	`Clc1c2Oc3c(Oc2c(Cl)c(Cl)c1Cl)c(Br)c(Cl)c(Cl)c3Cl`		$1.18e+03$	$6.02e+02$	$4.92e+04$	$2.07e-09$	$2.38e-07$	$1.99e+02$	9.74	*No*
192	109302-40-1	`Clc1c(Cl)c2oc3c(Br)c(Cl)c(Cl)c(Cl)c3c2c(Cl)c1Cl`		$9.06e+02$	$1.22e+03$	$4.24e+04$	$1.35e-08$	$1.28e-06$	$1.07e+03$	9.12	*No*
193	141074-63-7	`OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F`		$2.61e+04$	$3.16e+00$	$1.17e+06$	$6.61e-08$	$7.06e-06$	$2.06e+01$	9.5	*No*