Appendix 1 List of PFOS, its salts and its precursors identified through Section 71 CEPA 1999 industry survey, CATABOL modelling, and expert judgment [a]

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
N/A	PFOS anion	1-Octanesulfonate,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	$C_8F_{17}SO_3^-$	-	-
1763-23-1	PFOS acid (perfluoro-octanesulfonic acid) (also called PFOSH)	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	$C_8F_{17}SO_3H$	Y	Y
2795-39-3	PFOS potassium (K^+) salt	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, potassium salt	$C_8F_{17}SO_3K$	Y	Y
29081-56-9	PFOS ammonium (NH_4^+) salt	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, ammonium salt	$C_8F_{17}SO_3NH_4$	Y	Y
29457-72-5	PFOS lithium (Li^+) salt	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, lithium salt	$C_8F_{17}SO_3Li$	Y	Y
70225-14-8	PFOS diethanolamine (DEA) salt	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, compd. with 2,2-iminobis[ethanol] (1:1)	$C_8F_{17}SO_3NH(CH_2CH_2OH)_2$	Y	Y
307-35-7	POSF	1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	$C_8F_{18}O_2S$	Y	Y
1691-99-2	N-EtFOSE alcohol	1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-	$C_{12}H_{10}F_{17}NO_3S$	Y	Y
4151-50-2	N-EtFOSA	1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	$C_{10}H_6F_{17}NO_2S$	Y	Y
24448-09-7	N-MeFOSE alcohol	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-N-methyl-	$C_{11}H_8F_{17}NO_3S$	Y	Y
31506-32-8	N-MeFOSA	1-Octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-methyl-	$C_9H_4F_{17}NO_2S$	Y	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
25268-77-3	N-MeFOSEA	2-Propenoic acid, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester	$C_{14}H_{10}F_{17}NO_4S$	Y	Y
423-82-5	N-EtFOSEA	2-Propenoic acid, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester	$C_{15}H_{12}F_{17}NO_4S$	Y	Y
2250-98-8		1-Octanesulfonamide, N,N',N''-[phosphinylidynetris(oxy-2,1-ethanediyl)]tris[N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	$C_{36}H_{27}F_{51}N_3O_{10}PS_3$	Y	Y
2991-51-7		Glycine, N-ethyl-N-[(heptadecafluorooctyl)sulfonyl]-, potassium salt	$C_{12}H_8F_{17}NO_4S{\cdot}K$	Y	Y
29117-08-6		Poly(oxy-1,2-ethanediyl), α-[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl]-ω-hydroxy-	$(C_2H_4O)_nC_{12}H_{10}F_{17}NO_3S$	could not be modelled	Y
30381-98-7		1-Octanesulfonamide, N,N-[phosphinicobis(oxy-2,1-ethanediyl)]bis[N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, ammonium salt	$C_{24}H_{19}F_{34}N_2O_8PS_2{\cdot}H_3N$	Y	Y
38006-74-5		1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl]amino]-N,N,N-trimethyl-, chloride	$C_{14}H_{16}F_{17}N_2O_2S{\cdot}Cl$	Y	Y
52550-45-5		Poly(oxy-1,2-ethanediyl), α-[2-[[(heptadecafluorooctyl)sulfonyl]propylamino]ethyl]-ω-hydroxy-	$(C_2H_4O)_nC_{13}H_{12}F_{17}NO_3S$	could not be modelled	Y
56773-42-3		Ethanaminium, N,N,N-triethyl-, salt with 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-1-octanesulfonic acid (1:1)	$C_8H_{20}N{\cdot}C_8F_{17}O_3S$	Y	Y
57589-85-2		Benzoic acid, 2,3,4,5-tetrachloro-6-[[[3-[[(heptadecafluorooctyl)sulfonyl]oxy]phenyl]amino]carbonyl]-, monopotassium salt	$C_{22}H_6Cl_4F_{17}NO_6S{\cdot}K$	Y	Y
67939-88-2		1-Octanesulfonamide, N-[3-(dimethylamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, monohydrochloride	$C_{13}H_{13}F_{17}N_2O_2S{\cdot}ClH$	Y	Y
67969-69-1		1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-[2-(phosphonooxy)ethyl]-, diammonium salt	$C_{12}H_{11}F_{17}NO_6PS_2{\cdot}H_3$	Y	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
			N		
68298-11-3		1-Propanaminium, 3-[[(heptadecafluorooctyl)sulfonyl](3-sulfopropyl)amino]-N-(2-hydroxyethyl)-N,N-dimethyl-, hydroxide, inner salt	$C_{18}H_{23}F_{17}N_2O_6S_2$	Y	Y
68298-62-4		2-Propenoic acid, 2-[butyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, telomer with 2-[butyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, methyloxirane polymer with oxirane di-2-propenoate, methyloxirane polymer with oxirane mono-2-propenoate and 1-octanethiol	$(C_{17}H_{16}F_{17}NO_4S \cdot C_{16}H_{16}F_{15}NO_4S \cdot W_{99} \cdot W_{99})_x \cdot C_8H_{18}S$	could not be modelled	Y
68298-78-2		2-Propenoic acid, 2-methyl-, 2-[[[[5-[[[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl ester, telomer with butyl 2-propenoate, 2-[[[[5-[[[2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[[[5-[[[2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethoxy]carbonyl]amino]-2-methylphenyl]amino]carbonyl]oxy]propyl 2-methyl-2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol	$(C_{28}H_{28}F_{17}N_3O_8S \cdot C_{27}H_{28}F_{15}N_3O_8S \cdot C_{26}H_{28}F_{13}N_3O_8S \cdot C_{25}H_{28}F_{11}N_3O_8S \cdot C_{24}H_{28}F_9N_3O_8S \cdot C_{14}H_{10}F_{17}NO_4S \cdot C_{13}H_{10}F_{15}NO_4S \cdot C_{12}H_{10}F_{13}NO_4S \cdot C_{11}H_{10}F_{11}NO_4S \cdot C_{10}H_{10}F_9NO_4S \cdot C_7H_{12}O_2)_x \cdot C_8H_{18}S$	could not be modelled	Y
68329-56-6		2-Propenoic acid, eicosyl ester, polymer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate,	$(C_{23}H_{44}O_2 \cdot C_{21}H_{40}O_2 \cdot C_{19}H_{36}O_2 \cdot C_{14}H_{10}F_{17}N$	could not be modelled	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
		hexadecyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and octadecyl 2-propenoate	$O_4S{\cdot}C_{13}H_{10}F_{15}NO_4S{\cdot}C_{12}H_{10}F_{13}NO_4S{\cdot}C_{11}H_{10}F_{11}NO_4S{\cdot}C_{10}H_{10}F_9NO_4S)_x$		
68555-90-8		2-Propenoic acid, butyl ester, polymer with 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate and 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate	$(C_{14}H_{10}F_{17}NO_4S{\cdot}C_{13}H_{10}F_{15}NO_4S{\cdot}C_{12}H_{10}F_{13}NO_4S{\cdot}C_{11}H_{10}F_{11}NO_4S{\cdot}C_{10}H_{10}F_9NO_4S{\cdot}C_7H_{12}O_2)_x$	could not be modelled	Y
68555-91-9		2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, polymer with 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and octadecyl 2-methyl-2-propenoate	$(C_{22}H_{42}O_2{\cdot}C_{16}H_{14}F_{17}NO_4S{\cdot}C_{15}H_{14}F_{15}NO_4S{\cdot}C_{14}H_{14}F_{13}NO_4S{\cdot}C_{13}H_{14}F_{11}NO_4S{\cdot}C_{12}H_{14}F_9NO_4S)_x$	could not be modelled	Y
68555-92-0		2-Propenoic acid, 2-methyl-, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester, polymer with 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and octadecyl 2-methyl-2-propenoate	$(C_{22}H_{42}O_2{\cdot}C_{15}H_{12}F_{17}NO_4S{\cdot}C_{14}H_{12}F_{15}NO_4S{\cdot}C_{13}H_{12}F_{13}NO_4S{\cdot}C_{12}H_{12}F_{11}NO_4S{\cdot}C_{11}H_{12}F_9NO_4S)_x$	could not be modelled	Y
68586-14-1		2-Propenoic acid, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester, telomer with 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, α-(2-methyl-1-oxo-2-propenyl)-ω-hydroxypoly(oxy-1,2-ethanediyl), α-(2-methyl-1-oxo-2-propenyl)-ω-[(2-methyl-1-	$(C_{14}H_{10}F_{17}NO_4S{\cdot}C_{13}H_{10}F_{15}NO_4S{\cdot}C_{12}H_{10}F_{13}NO_4S{\cdot}C_{11}H_{10}F_{11}NO_4S{\cdot}C_{10}H_{10}F_9NO_4S{\cdot}(C_2H_4O)_nC_8H_{10}O_3{\cdot}(C_2H_4$	could not be modelled	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
		oxo-2-propenyl)oxy]poly(oxy-1,2-ethanediyl), 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 1-octanethiol	$O)_nC_4H_6O_2)_x \cdot C_8H_{18}S$		
68649-26-3		1-Octanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-, reaction products with N-ethyl-1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-1-butanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-1-heptanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N-(2-hydroxyethyl)-1-hexanesulfonamide, N-ethyl-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-N-(2-hydroxyethyl)-1-pentanesulfonamide, polymethylenepolyphenylene isocyanate and stearyl alc.	$(C_{18}H_{38}O \cdot C_{12}H_{10}F_{17}NO_3S \cdot C_{11}H_{10}F_{15}NO_3S \cdot C_{10}H_{10}F_{13}NO_3S \cdot .C\text{-}H_{10}F_{11}NO_3S \cdot C_8H_{10}F_9NO_3S \cdot \text{Unspecified})_x$	could not be modelled	Y
68867-62-9		2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, telomer with 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 1-octanethiol and α-(1-oxo-2-propenyl)-ω-methoxypoly(oxy-1,2-ethanediyl)	$(C_{16}H_{14}F_{17}NO_4S \cdot C_{15}H_{14}F_{15}NO_4S \cdot C_{14}H_{14}F_{13}NO_4S \cdot C_{13}H_{14}F_{11}NO_4S \cdot C_{12}H_{14}F_9NO_4S \cdot (C_2H_4O)_nC_4H_6O_2)_x \cdot C_8H_{18}S$	could not be modelled	Y
68877-32-7		2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester, polymer with 2-[ethyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate, 2-[ethyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-methyl-2-propenoate and 2-methyl-1,3-butadiene	$(C_{16}H_{14}F_{17}NO_4S \cdot C_{15}H_{14}F_{15}NO_4S \cdot C_{14}H_{14}F_{13}NO_4S \cdot C_{13}H_{14}F_{11}NO_4S \cdot C_{12}H_{14}F_9NO_4S \cdot C_5H_8)_x$	could not be modelled	Y
68891-96-3		Chromium, diaquatetrachloro[μ-[N-ethyl-N-[(heptadecafluorooctyl)sulfonyl]glycinato-O':O"]]μ-hydroxybis(2-methylpropanol)di-	$C_{18}H_{28}Cl_4Cr_2F_{17}NO_9S$	Y	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
68958-61-2		Poly(oxy-1,2-ethanediyl), α-[2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl]-ω-methoxy-	$(C_2H_4O)_nC_{13}H_{12}F_{17}NO_3S$	could not be modelled	Y
70776-36-2		2-Propenoic acid, 2-methyl-, octadecyl ester, polymer with 1,1-dichloroethene, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, N-(hydroxymethyl)-2-propenamide, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate and 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate	$(C_{22}H_{42}O_2 \cdot C_{14}H_{10}F_{17}NO_4S \cdot C_{13}H_{10}F_{15}NO_4S \cdot C_{12}H_{10}F_{13}NO_4S \cdot C_{11}H_{10}F_{11}NO_4S \cdot C_{10}H_{10}F_9NO_4S \cdot C_4H_7NO_2 \cdot C_2H_2Cl_2)_x$	could not be modelled	Y
71487-20-2		2-Propenoic acid, 2-methyl-, methyl ester, polymer with ethenylbenzene, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl 2-propenoate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl 2-propenoate and 2-propenoic acid	$(C_{14}H_{10}F_{17}NO_4S \cdot C_{13}H_{10}F_{15}NO_4S \cdot C_{12}H_{10}F_{13}NO_4S \cdot C_{11}H_{10}F_{11}NO_4S \cdot C_{10}H_{10}F_9NO_4S \cdot C_8H_8 \cdot C_5H_8O_2 \cdot C_3H_4O_2)_x$	could not be modelled	Y
92265-81-1		Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, chloride, polymer with 2-ethoxyethyl 2-propenoate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl 2-propenoate and oxiranylmethyl 2-methyl-2-propenoate	$(C_{14}H_{10}F_{17}NO_4S \cdot C_9H_{18}NO_2 \cdot C_7H_{12}O_3 \cdot C_7H_{10}O_3 \cdot Cl)_x$	N	Y
94313-84-5		Carbamic acid, [5-[[[2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethoxy]carbonyl]amino]-2-methylphenyl]-, 9-octadecenyl ester, (Z)-	$C_{38}H_{50}F_{17}N_3O_6S$	Y	Y
98999-57-6		Sulfonamides, C_{7-8}-alkane, perfluoro, N-methyl-N-[2-[(1-oxo-2-propenyl)oxy]ethyl], polymers with 2-ethoxyethyl acrylate, glycidyl methacrylate and N,N,N-trimethyl-2-[(2-methyl-1-oxo-propenyl)oxy]ethanaminium chloride	$(C_{14}H_{10}F_{17}NO_4S \cdot C_9H_{18}NO_2 \cdot C_7H_{12}O_3 \cdot C_7H_{10}O_3 \cdot Cl)_x$	could not be modelled	Y
178094-69-4		1-Octanesulfonamide, N-[3-(dimethyloxidoamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-, potassium salt	$C_{13}H_{12}F_{17}N_2O_3S \cdot K$	Y	Y
N/A		2-(Perfluoro-N-methyl-C_{4-8}-1-alkanesulfonamido)ethyl esters of trimers of C_{18} unsaturated fatty acids	N/A	could not be modelled	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
68909-15-9		2-Propenoic acid, eicosyl ester, polymers with branched octyl acrylate, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl acrylate, 2-[methyl[(nonafluorobutyl)sulfonyl]amino]ethyl acrylate, 2-[methyl[(pentadecafluoroheptyl)sulfonyl]amino]ethyl acrylate, 2-[methyl[(tridecafluorohexyl)sulfonyl]amino]ethyl acrylate, 2-[methyl[(undecafluoropentyl)sulfonyl]amino]ethyl acrylate, polyethylene glycol acrylate Me ether and stearyl acrylate	$(C_{23}H_{44}O_2 \cdot C_{21}H_{40}O_2 \cdot C_{14}H_{10}F_{17}NO_4S \cdot C_{13}H_{10}F_{15}NO_4S \cdot C_{12}H_{10}F_{13}NO_4S \cdot C_{11}H_{10}F_{11}NO_4S \cdot C_{10}H_{10}F_9NO_4S \cdot (C_2H_4O)_nC_4H_6O_2 \cdot \text{Unspecified})_x$	could not be modelled	Y
148684-79-1		Sulfonamides, C_{4-8}-alkane, perfluoro, N-(hydroxyethyl)-N-methyl, reaction products with 1,6-diisocyanatohexane homopolymer and ethylene glycol	N/A	could not be modelled	Y
30295-51-3		1-Octanesulfonamide, N-[3-(dimethyloxidoamino)propyl]-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	N/A	Y	Y
91081-99-1		Sulfonamides, C_{4-8}-alkane, perfluoro, N-(hydroxyethyl)-N-methyl, reaction products with epichlorohydrin, adipates (esters)	N/A	could not be modelled	Y
N/A		Fatty acids, C_{18}-unsatd., dimers, 2-[methyl[(perfluoro-C_{4-8}-alkyl)sulfonyl]amino]ethyl esters	N/A	Y	Y
68081-83-4		Carbamic acid, (4-methyl-1,3-phenylene)bis-, bis[2-[ethyl[(perfluoro-C_{4-8}-alkyl)sulfonyl]amino]ethyl] ester		Y	Y
68608-14-0		Sulfonamides, C_{4-8}-alkane, perfluoro, N-ethyl-N-(hydroxyethyl), reaction products with 1,1'-methylenebis[4-isocyanatobenzene]	$C_{15}H_{10}N_2O_2 \cdot \text{Unspecified}$	Y	Y
376-14-7		2-Propenoic acid, 2-methyl-, 2-[ethyl[(heptadecafluorooctyl)sulfonyl]amino]ethyl ester	$C_{16}H_{14}F_{17}NO_4S$	Y	Y
14650-24-9		2-Propenoic acid, 2-methyl-, 2-[[(heptadecafluorooctyl)sulfonyl]methylamino]ethyl ester	$C_{15}H_{12}F_{17}NO_4S$	Y	Y
94133-90-1		1-Propanesulfonic acid, 3-[[3-(dimethylamino)propyl][(heptadecafluorooctyl)sulfonyl]amino]-2-hydroxy-, monosodium salt	$C_{16}H_{19}F_{17}N_2O_6S_2 \cdot Na$	Y	Y
127133-66-8		2-Propenoic acid, 2-methyl-, polymers with Bu methacrylate, lauryl methacrylate and 2-[methyl[(perfluoro-C_{4-8}-alkyl)sulfonyl]amino]ethyl methacrylate	$(C_{16}H_{30}O_2 \cdot C_8H_{14}O_2 \cdot C_4H_6O_2)_x$	Y	Y
179005-06-2		Sulfonamides, C_{4-8}-alkane, perfluoro, N-[3-(dimethyloxidoamino)propyl], potassium salts	N/A	could not be modelled	Y

CAS No.	Common name	Chemical name	Molecular formula	PFOS Precursor (Catabol)[b]	PFOS Precursor (expert judgment)
179005-07-3		Sulfonamides, C_{4-8}-alkane, perfluoro, N-[3-(dimethyloxidoamino)propyl]	N/A	could not be modelled	Y
ROF		Residual Organic Fluorochemicals (impurities)	N/A	Y	Y

[a] Notes:
1. References: Mekenyan *et al*. (2002); Purdy (2002).
2. N/A = not available; Bu = butyl; Et = ethyl; Me = methyl.
3. This list is not necessarily an exhaustive list of all possible PFOS precursors.

[b] For each substance modelled, CATABOL generates a microbial metabolic pathway tree based upon the parent "query" structure and a prediction for biodegradability. The metabolic pathway tree module is based on a training data set primarily from the University of Minnesota Biocatalysis/Biodegradation database (UM-BBD) and expert knowledge. The metabolic tree contains the products of microbial biodegradation from the parent compound down to carbon dioxide and water or stable metabolites. Some of the chemicals could not be modelled by CATABOL due to the lack of SMILES notation. The biodegradation simulator is based on a database of 742 substances tested by CITI (1992) using the Modified MITI Test (I), which follows the OECD 301C test methods and is one of six methods approved by the OECD for ready biodegradability. A more complete description of the CATABOL modelling is provided in Robinson (2002).