

名称	OASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 復帰突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性
Fluorotelomer alcohol 4:2	2043-47-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
Fluorotelomer alcohol 6:2	647-42-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives	TA1535,TA1537,TA98,TA100,WP2uvrA(±S9)Negative//TA1535, TA1537, TA98,TA100, WP2 uvrA (±S9) Negative	CHO(±S9) Negative;H PBL(±S9) Negative// mouse lymphoma LS178Y cells +S9;Positive (±S9) Negative// human peripheral blood lymphocytes Negative(±S9); Chinese hamster	LS178Y (± S9) Negative// mouse lymphoma LS178Y cells Negative(± S9) Ambiguous (+S9)Negative(-S9)										Or(10) WU BRラット雄 Negative			
Fluorotelomer alcohol 8:2	678-39-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives	TA98, TA100, TA1535, TA1537, WP2uvrA, TA98, TA100, WGP2uvrA pM101(±S9) Negative														腫瘍発生なし、肝腫瘍促進活性なし	
追加 Fluorotelomer alcohol 10:2	865-86-1		No alert found	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives	TA98, TA100, WP2uvrA pM101(±S9) Negative															
6:1 Fluorotelomer alcohol	375-82-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
9:1 Fluorotelomer alcohol	307-37-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
11,11,11-Perfluoro-1-octanol	10331-08-5		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by I5S	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by I5S	In vivo mutagenicity (Micronucleus) alerts by I5S	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 糖脂形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
5:1 Fluorotelomer alcohol	423-46-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
1H,1H,11H-Eicosafluoro-1-undecanol	307-70-0		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
1H,1H,5H-Perfluoropentanol	355-80-6		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
3-(Perfluorooctyl)propanol	1651-41-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
1H,1H-Perfluoro-1-pentanol	355-28-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
1H,1H-Hexadecafluoro-1-nonanol	378-18-1		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																
3-(Perfluorobutyl)propanol	83310-97-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbons																

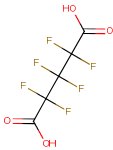
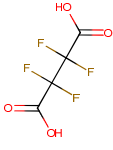
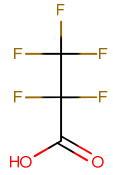
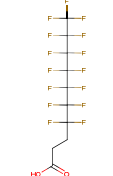
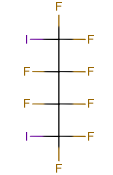
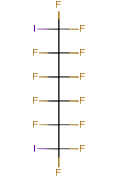
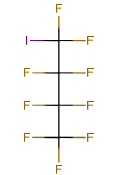
名称	QASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
3:1 Fluorotelomer alcohol	375-01-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
2:1 Fluorotelomer alcohol	422-05-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives		Chinese hamster Lung (± SSI)Negative														
6- (Perfluorohexyl)hexanol	161981-35-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
Fluorotelomer alcohol 3:2	755-40-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
7:3 Fluorotelomer alcohol	25600-66-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
7:1 Fluorotelomer alcohol	307-30-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																
4:4 Fluorotelomer alcohol	3792-02-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluor ocarbon derivatives																

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3- (Perfluoropropyl)propanol	678-02-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
Fluorotelomer alcohol 2,2	54949-74-5		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
3- (Perfluoroheptyl)propanol	80806-68-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
3- (Perfluoroethyl)propanol	148043-73-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
8:1 Fluorotelomer alcohol	423-56-3		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
11:1 Fluorotelomer alcohol	423-65-4		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																
Perfluorobutanol	3056-01-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives																

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1H,1H,7H-Dodecafluoro-1-heptanol	335-99-9			No alert found	No alert found	No alert found	Acylation/Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Perfluorocarbon derivatives															
Perfluorooctanoic acid	2706-90-3			No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives															
Perfluorooctanoic acid	335-67-1		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives	TA98,TA100,TA102,TA104 (±S8) Negative, [NH4+塩] TA98,TA100,TA1535,TA1537,TA1538, S.verruisat;D4,WP2uvrA(±S8);Negative;Na+塩 TA98,TA100,TA1535,TA1537,WP2uvrA (±S8) Negative	[CHO(+S8) Negative [NH4+塩];ヒトリンパ球, CHO(+S8) Negative Na+塩]	TK cell Positive	Tkcell Negative				[C3H 10T1/2細胞 Negative [NH4+塩]	C57BL/6J マウス雄 網状赤血球、脾臓リンパ球 Negative [CD-11cR] マウス雄雄 骨髄 Negative [NH4+塩;Na 塩]	雄ラット (G+1COBS-CD/SD)- Sames and Doolittle (1986)	C57BL/6J マウス雄 肝細胞、精巣細胞 Negative			肝発がん性に関しては、PPARα、CAR等の核内受容体の活性化の誘起、PPARαの活性化の関与が示唆、PFOAによるウイザイクヒ細胞腫瘍は高用量での誘発であった	
Perfluorooctanoic acid	375-85-9		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives	TA98,TA100,TA1535,TA1537,TA1538 (±S8) Negative			V79;Negative											
Perfluorobutanoic acid	375-22-4			No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives	TA98,TA100,TA1535,TA1538,TA1539 (±S8) Negative			V79 (±S8) Negative						Fischer344 rat, LI, KI Negative					
Perfluorooctanoic acid	307-24-4		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives	TA98,TA100,WP2uvrA,TA98,TA100,TA1535,TA1537,WP2uvrA,TA98,TA100,TA1535,TA1537,TA1538 (±S8) Negative	ヒト末梢血リンパ球(±S8) Negative	HepG2 Negative	V79(±S8) Negative				SDラット末梢血 雄 Equivocal/ 雄Negative						発がん兆候なし	
Perfluorooctanoic acid	678-45-5		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found		Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives															

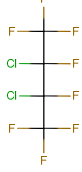
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by IIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by IIS	In vivo mutagenicity (Micronucleus) alerts by IIS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
3,3-Fluorotelomer carboxylic acid	356-02-5		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Potassium perfluorooctanoate	2395-00-8		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Perfluorooctanedioic acid	23453-64-7		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether; Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
2H,2H,3H,3H-Perfluorooctanoic acid	914637-49-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Perfluorooctanedioic acid	336-08-3		Phthalate (or butyl) diesters and monoesters (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether; Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Sodium perfluorooctanoate	335-95-5		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Perfluorooctanedioic acid	307-78-8		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether; Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																

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8:3 Fluorotelomer carboxylic acid	34598-33-9		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
4H- Perfluorobutanoic acid	678-12-9		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
7H- Perfluoroheptanoic acid	1546-95-8		Perfluorooctanoic acid (PFOA) (Nongenotox): Structural alert for nongenotox carcinogenicity	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
3- (Perfluorohexyl)propanoic acid	27854-30-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
8H- Perfluorooctanoic acid	13973-14-3		Perfluorooctanoic acid (PFOA) (Nongenotox): Structural alert for nongenotox carcinogenicity	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Ammonium perfluorooctanoate	3825-26-1		Perfluorooctanoic acid (PFOA) (Nongenotox): Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
3- (Perfluorobutyl)propanoic acid	80705-13-1		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																

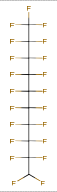
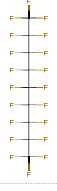
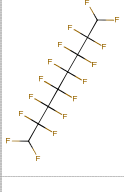
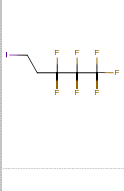
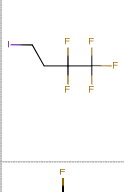

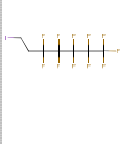
名称	OASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 糖脂質置換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メット試験	In vivo コメット試験	In vivo 突然変異	発がん性
Perfluoropentanoic acid	378-73-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Halooether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																	
Perfluorobutanedioic acid	377-38-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Halooether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																	
Perfluoropropanoic acid	422-64-0		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Halooether Reactive Functional Groups	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																	
3-(Perfluoroheptyl)propanoic acid	812-70-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOA)Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																	
Perfluoro-1,4-diiodobutane	375-50-8		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives	TA1535, TA1537, TA98, TA100, TA102, WP2 (±S9) Negative	peripheral human lymphocyte ± (±S9) Negative															
1,6-Diiodoperfluorohexane	375-39-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives	TA1535, TA1537, TA98, TA100, TA102 (±S9) Negative																
Nonafluoro-1-iodobutane	423-39-2		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives	TA1535, TA1537, TA98, TA100 (±S9) Negative																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by IIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by IIS	In vivo mutagenicity (Micronucleus) alerts by IIS	Organic functional groups	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Heptafluoropropyl iodide	754-34-7		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1,6-Dibromododecafluorohexane	918-22-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
2-Iodoheptafluorobutane	375-51-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1-Bromoheptafluorobutane	375-49-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1-Bromoheptafluoropropane	422-85-5		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1,8-Diiodooctane	335-70-6		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1-Chloro-6-iodoheptafluorohexane	16486-97-8		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															

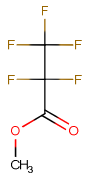
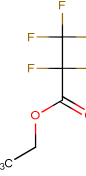

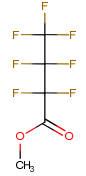
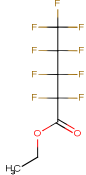
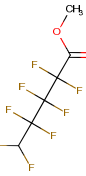
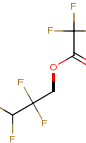
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by EIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーム試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
1-Iodopentadecafluoroheptane	335-58-0		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1-Iodoperfluoropentane	638-79-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
Heptafluoro-2-iodopropane	677-69-0		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
1,2-Dibromohexafluoropropane	661-95-0		No alert found	No alert found	SN2;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihalooalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihalooalkanes	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
Perfluorodecane	307-43-7		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
Perfluoro-1-iodohexane	355-43-1		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															
Perfluorohexyl bromide	335-56-8		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives															

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 体異常試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性
Perfluorohexyl chloride	355-41-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																	
Perfluorodecyl iodide	423-62-1		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																	
1-Bromopentafluoroheptane	375-88-2		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																	
1,4-Dibromo-1,1,2,2-tetrafluorobutane	18599-20-7		Aliphatic halogens (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2;SN2 >> SN2 at an sp3 Carbon atom;SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																	
2,3-Dichlorooctafluorobutane	355-20-4		No alert found	No alert found	SN2;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihalooalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihalooalkanes	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																	
追加 pentafluoroiodoethane	354-64-3		No alert found	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives	Positive(NBS)																
1H-Perfluorohexane	355-37-3		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives	TA1535, TA1537,TA98,TA100, WP2 (±S8) Negative	CHL Cells clone No. 11 (±S8) Negative	mouse lymphoma L5178Y (±S8) Negative														

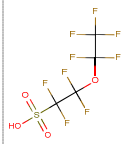
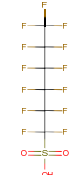
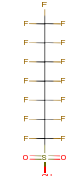
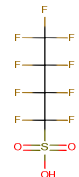
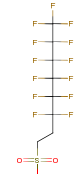

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーム試験	in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	in vitro HprtT試験	in vitro 不 定期DNA合 成試験	in vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不 定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo突然変異	発がん性	
(Perfluoro- <i>n</i> -hexyl)ethane	80793-17-5		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives	TA1535, TA1537,TA98,TA100, WP2 (±S9) Negative	Chinese hamster lung fibroblasts (V79) (±S9) Negative															
Perfluorooctane	307-34-6		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives	TA1535,TA1537,TA98,TA100,WP2 (±S9)Negative	Chinese Hamster Lung Cells (±S9)Negative															
1-(Perfluorohexyl)octane	13331-77-8		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives																	
1,1,2-Tetrafluoro-3-iodopropane	679-67-8		Aliphatic halogens (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halide;Perfluorocarbon derivatives																	
Heptafluorobutyl iodide	374-99-1		Aliphatic halogens (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halide;Perfluorocarbon derivatives																	
(Perfluoromethyl)methyl iodide	354-69-8		Aliphatic halogens (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halide;Perfluorocarbon derivatives																	
1H,9H-Perfluorohexane	336-07-2		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives																	





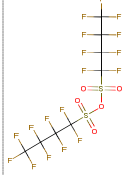
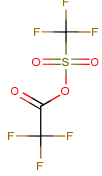

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 変異試験	遺伝毒性 in vitro 変異試験	遺伝毒性 in vitro コマンド試験	遺伝毒性 in vitro DNA 損傷試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コマンド試験	In vivo 突然変異	発がん性
1-H-Perfluorodecane	375-97-3		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halidePerfluorocarbon derivatives														
Perfluorononane	375-96-2		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halidePerfluorocarbon derivatives														
1H,8H-Perfluorooctane	307-99-3		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halidePerfluorocarbon derivatives														
3,2-Fluorotetramer iodide	1513-88-8		Aliphatic halogens (Genotox): Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2:SN2 >> SN2 at an sp3 Carbon atom:SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halidePerfluorocarbon derivatives														
2,2-Fluorotetramer iodide	40723-80-6		Aliphatic halogens (Genotox): Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2:SN2 >> SN2 at an sp3 Carbon atom:SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halidePerfluorocarbon derivatives														
1-Isodecyl-1H,1H,2H,2H-perfluoroheptane	375-93-7		No alert found	No alert found	No alert found	AcylationAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halidePerfluorocarbon derivatives														
1-Isodecyl-1H,1H,2H,2H-perfluoroheptane	1682-31-1		Aliphatic halogens (Genotox): Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2:SN2 >> SN2 at an sp3 Carbon atom:SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halidePerfluorocarbon derivatives														

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 糖形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluorodecane	307-45-9			No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide/Perfluorocarbon derivatives																
1-Iodo-1H,1H,2H,2H-perfluorononane	2043-52-9		Aliphatic halogens (Genotox) Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2:SN2 >> SN2 at an sp3 Carbon atom:SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkyl halide/Perfluorocarbon derivatives																
(Perfluoro-)-octylethane	77117-48-7			No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide/Perfluorocarbon derivatives																
Methyl 4H-perfluorobutanoate	356-32-1			No alert found	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl Halides:Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide/Carboxylic acid ester/Perfluorocarbon derivatives															
Methyl perfluoropentanoate	13038-26-1			No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide/Carboxylic acid ester/Perfluorocarbon derivatives																
Methyl perfluorohexanoate	424-18-0		Perfluorooctanoic acid (PFOA) (Nongenotox): Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide/Carboxylic acid ester/Perfluorocarbon derivatives																
Ethyl 9H-octadecanenoate	2785-50-8			No alert found	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl Halides:Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide/Carboxylic acid ester/Perfluorocarbon derivatives															

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by EIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複製突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Methyl pentafluoropionate	378-75-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluoropropionate	426-65-3		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Diethyl perfluoroglutarate	424-40-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Methyl perfluorobutanoate	356-24-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluoropentanoate	424-36-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Methyl 9H-perfluoropentanoate	54822-22-9		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
2,2,3,3-Tetrafluoropropyl trifluoroacetate	107551-72-4		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Methyl 2H,2H,3H,3H-perfluoroheptanoate	132424-36-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluorooctanoate	3108-24-5		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluorononanoate	30377-52-7		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluoroheptanoate	41430-70-0		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Methyl perfluorooctanoate	376-27-2		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
Ethyl perfluorobutanoate	356-27-4		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
8,2 Fluorotelomer sulfonic acid	39108-34-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluoro carbon derivatives;Sulfonic acid;Surfactants - Anionic																

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4,2-Fluorotelomer sulfonic acid	757124-72-4		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																
Perfluoro-2-ethoxyethanesulfonic acid	113507-82-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether (Reactive Functional Groups)	No alert found	H+acceptor-path3-H+acceptor	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																
Perfluorooxanesulfonic acid	355-46-4		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic			温度依存的な振動を示すが、温度依存性は明確ではない												実験動物では情報なし	
Perfluoroheptanesulfonic acid	375-92-8		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																
Perfluorobutanesulfonic acid	375-73-5		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic	TA100 Negative, TA98 Equivalent (±S8)/TA1535, TA1537, TA98,TA100, WP2 unrA (±S8) Negative		HepG2 Negative						rat 雄 終末 精血 Negative						認められず	
6,2-Fluorotelomer sulfonic acid	27619-97-2		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic	TA1535, TA1537, TA98,TA100, TA102 (±S8) Negative	Chinese hamster Ovary (CHO)(±S8) Positive													Cr(CD)SD)ラット肝、胃 Negative/(TG489濃度 GLP適合) カリウム塩	
Potassium perfluorobutanesulfonate	29420-49-3		No alert found	No alert found	No alert found	No alert found		No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic	TA1535, TA1537,TA98,TA100, TA102, WP2 unrA (±S8) Negative	Chinese hamster Ovary, lung fibroblasts (V79) (±S8) Negative														

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Trifluoromethanesulfonic acid	1493-13-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic	TA1535, TA1537,TA98,TA100, WP2uvrA (±S8) Negative	CHL Cells clone No. 11 (±S8) Negative	mouse lymphoma L5178Y (±S8) Negative													
Potassium perfluorooctanesulfonate	2795-39-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic	ネズミ胚肝臓、肺、大腸臓(±S8) Negative	ヒト全血培養リンパ球(±S8) Negative						ラット肝細胞移植細胞 Negative	mouse骨髄 Negative						SDラット肝細胞移植有意に増加。肝臓腫瘍有意に増加。甲状腺線細胞腫瘍+濾胞癌を合わせて有意に発生率上昇。乳腺組織腫瘍または乳腺線腫瘍	
Perfluorooctanesulfonic acid	1763-23-1		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic		Negative	Hep G2 濃度依存性は明確ではない positive あり	Negative				Positive(1件 ATSDR)	Negativeとされているが以下の報告あり gpt delta 1gマウス腫瘍 Negative; Wistarラット骨髄細胞軽度増加; Wistarラット末梢血 Positive					Wistarラットコメットスコア増加; Wistarラット末梢血 Positive	gpt delta 1gマウス腫瘍毒性/発がん性試験において、肝臓の増加傾向あり	動物の慢性毒性/発がん性試験に有意な増加あり
Potassium perfluorohexanesulfonate	3871-99-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic																
Perfluorobutanesulfonic anhydride	36913-91-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H+acceptor-path3-H+acceptor	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic																
Trifluoroacetyl triflate	68602-57-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H+acceptor-path3-H+acceptor	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic																
Sodium perfluorodecane sulfonate	2806-15-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	(PFOS)Alkyl halide;Perfluorocarbons;Sulfonic acid;Surfactants - Anionic																

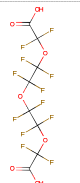
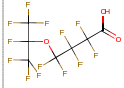
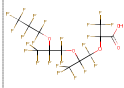
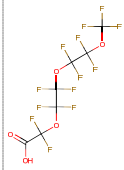
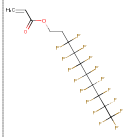
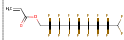
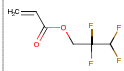
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Perfluorooctanesulfonate	45298-90-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	PFOS)Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																
Ethyl perfluorobutyl ether	163702-05-4		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
Difluoromethyl 1H,1H-perfluoropropyl ether	56860-81-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
Methyl 1H,1H-perfluoropropyl ether	378-16-5		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
1H,1H,5H-Perfluoropentyl-1,1,2,2-tetrafluoroethyl ether	16627-71-7		No alert found	Radical/Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical/Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
Perfluorobutyl methyl ether	163702-07-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
2H-Perfluoro-5-methyl-3,6-dioxanone	3330-14-1		No alert found	No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor;path3-H+ acceptor	Alkyl halide;Ether moiety;Perfluorocarbon derivatives															

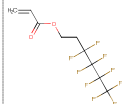


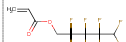
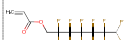

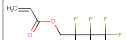
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	遺伝毒性 in vitro HPRIT試験	遺伝毒性 in vitro 不定期DNA合成試験	遺伝毒性 in vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性	
Di(2,2,3,3-tetrafluoropropyl) ether	35042-99-0		No alert found	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
(2H-Perfluoroethyl) (1H,1H,3H-perfluoropropyl) ether	16627-68-2		No alert found	Radical:Radical >> ROS formation after GSH depletion:Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical:Radical >> ROS formation after GSH depletion:Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation:Acylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
2,2,3,3-Tetrafluoropropyl ether	82914-35-0		No alert found	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
Methyl 2H,2H-perfluorobutyl ether	376-98-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
Methyl 3H-perfluoropropyl ether	56850-25-4		No alert found	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes:SN1 >> Carbocation Ion Formation:SN1 >> Carbocation Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
Perfluoro-3-(1H-perfluoroethoxy)propane	3330-15-2		No alert found	No alert found	No alert found	SN1:SN1 >> Carbocation Ion Formation:SN1 >> Carbocation Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																	
1,2-bis(1,1,2,2-Tetrafluoroethoxy)ethane	358-39-4		No alert found	Radical:Radical >> ROS formation after GSH depletion:Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical:Radical >> ROS formation after GSH depletion:Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation:Acylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halideEther moietyPerfluorocarbon derivatives																	

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by EIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
(1H,1H-Perfluoroethyl)(2H-perfluoroethyl) ether	406-78-0		No alert found	RadicalRadical >> ROS formation after GSH depletionRadical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	RadicalRadical >> ROS formation after GSH depletionRadical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives:SN2:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	AcylationAcylation >> P450 Mediated Activation to Acyl Halides >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halideEther moietyPerfluorocarbon derivatives																
7H-Perfluorohepta nyl chloride	41405-35-0		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halideAcylation >> P450 Mediated Activation to Acyl HalidesAcylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																
Perfluoronona nyl chloride	52447-23-1		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																
Perfluorooctan oyl fluoride	335-66-0		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																
Hexafluorooctan yl chloride	678-77-3		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																
Perfluorooctadecan oyl chloride	335-66-1		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																
Pentafluorooctadecan oyl chloride	335-64-8		Acyl halides (Genotox):Stru ctural alert for genotoxic carcinogenicity	No alert found	SN2:SN2 >> Direct acylation involving a leaving group:SN2 >> Direct acylation involving a leaving group >> Acyl Halides	AcylationAcylation >> Direct Addition of an Acyl HalideAcylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halideAlkyl halidePerfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複相突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluoroglutaryl difluoride	678-78-4		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
2,2-Bis(trifluoromethyl)propionyl fluoride	1735-87-1		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
5H-Octafluoropentanoyl fluoride	813-03-6		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
Perfluorooctanoyl chloride	52447-22-0		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
(Perfluorooctyl)propanoyl chloride	89373-67-1		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
Heptafluorobutryl Chloride	375-16-6		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorocarbon derivatives																
Perfluoro-3,6-dioxahexanoic acid	151772-58-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H ⁺ -acceptor;path3-H ⁺ -acceptor	(GenX)Alkyl halide;Carbonyl is acid;Ether moiety;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by IIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by IIS	In vivo mutagenicity (Micronucleus) alerts by IIS	Organic functional groups	遺伝毒性 in vitro 複製突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluoro(4-methoxybutanoic acid)	863090-89-5		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															
Perfluoro(3-methoxypropanoic acid)	377-73-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															
Perfluoro-2-methyl-3-octahexanoic acid	13252-13-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives	*アンモニウム塩のみ(CAS62037-80-3)	*アンモニウム塩のみ	*アンモニウム塩のみ					*アンモニウム塩のみ		*アンモニウム塩のみ	*アンモニウム塩のみ	*アンモニウム塩のみ			*アンモニウム塩のみ
Perfluoro-2,5-dimethyl-3,6-dioxanonanoic acid	13252-14-7		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															
Perfluoro-3,6-dioxaoctane-1,8-dioic acid	55621-21-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															
Perfluoro-3,6-trioxatridecanoic acid	330562-41-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															
Perfluoro-3,6-dioxadecanoic acid	137780-69-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives															

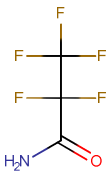
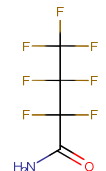
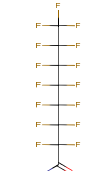
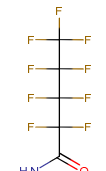
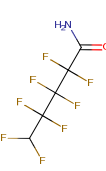
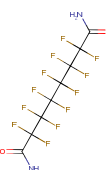
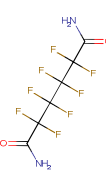
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluoro-3,6,9-trioxadecane-1,11-dioic acid	55621-18-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives																
Perfluoro-4-isopropoxybutanoic acid	801212-59-9		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives																
Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic) acid	65294-16-8		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives																
Perfluoro-3,6,9-trioxadecanoic acid	151772-59-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	(GenX)Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives																
2-(Perfluorooctyl)ethyl acrylate	27805-45-9		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives																
1H,1H,9H-Perfluorononyl acrylate	4180-26-1		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives																
2,2,3,3-Tetrafluoropropyl acrylate	7383-71-3		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複発突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマテスト	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メント試験	In vivo 突然変異	発がん性
Z- (Perfluorobutyl)ethyl acrylate	52591-27-2		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
1H,1H- Perfluorooctyl acrylate	307-98-2		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
1H,1H,5H,9H- Perfluoro-1,5-pentenediol diacrylate	678-95-5		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
1H,1H,5H- Perfluoropentyl acrylate	376-84-1		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
(6H- Perfluorohexyl)methyl acrylate	2993-85-3		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
1H,1H,6H,9H- Perfluorohexan e-1,6-diol diacrylate	2264-01-9		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																
1H,1H- Perfluorobutyl acrylate	424-64-6		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluoro carbon derivatives																

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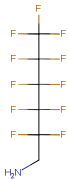

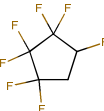
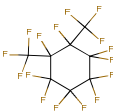
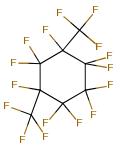

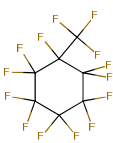
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
(Perfluoroheptyl)methyl methacrylate	3534-23-4		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
(Perfluorohexyl)methyl methacrylate	48076-44-4		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
1H,1H,7H-Perfluoroheptyl methacrylate	2261-99-6		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
1H,1H,2H,2H-Perfluorohexyl methacrylate	1799-94-4		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
Perfluorooctadecanoic acid	72629-94-8		Perfluorooctadecanoic acid (PFDA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives;Surfactants - Anionic																
Perfluorotetradecanoic acid	376-06-7		Perfluorooctadecanoic acid (PFDA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives;Surfactants - Anionic	TA100, TA1535, TA98, TA1538, WP2uvrA	CHL-1/JU (±S9) Negative// Chinese hamster lung cells (±S9) Negative														
Perfluoroundecanoic acid	2058-94-8		Perfluorooctadecanoic acid (PFDA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives;Surfactants - Anionic	TA100, TA1535, TA98, TA1537, WP2uvrA	CHL-1/JU (±S9) Positive// Chinese hamster lung cells (±S9) Positive	HepG2 Negative													

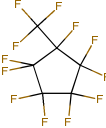
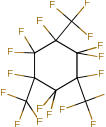
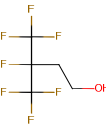
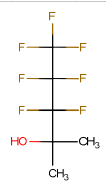

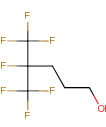
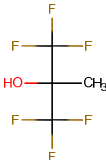
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification (Ames test) alerts by ISS	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 復帰突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	In vitro Hprt試験	In vitro 不定期DNA合成	In vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
追加	Perfluorooctadecanoic acid	67805-19-5		Perfluorooctadecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation>> Schiff base formation by aldehyde formed after metabolic activation>> Geminal Polyhaloalkane Derivatives:Radical>> Radical mechanism via ROS formation (indirect)>> Radical mechanism via ROS formation (indirect)>> Geminal Polyhaloalkane Derivatives:SN2,SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation>> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation>> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic	TA100,TA1535,TA98,TA1537,WP2uvrA (±S9) Negative	CHL/ILU (±S9) Negative	Negative	Negative											
追加	Perfluorooctadecanoic acid	16517-11-6		Perfluorooctadecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation>> Schiff base formation by aldehyde formed after metabolic activation>> Geminal Polyhaloalkane Derivatives:Radical>> Radical mechanism via ROS formation (indirect)>> Radical mechanism via ROS formation (indirect)>> Geminal Polyhaloalkane Derivatives:SN2,SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation>> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation>> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic	TA100,TA1535,TA98,TA1537,WP2uvrA (±S9) Negative	CHL/ILU Weakly Positive	Negative	Negative											
追加	Perfluorododecanoic acid	307-55-1		Perfluorododecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation>> Schiff base formation by aldehyde formed after metabolic activation>> Geminal Polyhaloalkane Derivatives:Radical>> Radical mechanism via ROS formation (indirect)>> Radical mechanism via ROS formation (indirect)>> Geminal Polyhaloalkane Derivatives:SN2,SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation>> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation>> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic	TA98, TA100, TA1535, TA1538,TA1538,TA1538,TA98,TA100,WP2uvrA,µM101,TA98,TA100,TA1535,TA1538,WP2uvrA (±S9) Negative	CHL/ILU (±S9) Positive	HepG2 Negative	V79(±S8) Negative											
	Perfluorodecanoic acid	335-76-2		Perfluorodecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic	TA98,TA100,TA1535,TA1537,TA1538,WP2 uvrA (±S9) Negative/TA1535,TA1537,TA98,TA100 (±S9) Negative		V79(±S8) Negative						Harlan SD ラット末梢血 腫瘍 Negative						
	Perfluorononanoic acid	375-95-1		Perfluorononanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic	TA98,TA100,TA1535,TA1537,TA1538,TA98,TA100,WP2uvr2 (±S9) Negative	ヒト肝臓がん細胞 Modest increase at a cytotoxic conc.; HepG2細胞 Positive	V79(±S8) Negative	TK6細胞 Positive					Harlan SD ラット末梢血 腫瘍 Negative						
9H-Perfluorononanoic acid	76-21-1		Perfluorooctadecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic																
11-H-Perfluoroundecanoic acid	1765-48-6		Perfluorooctadecanoic acid (PFOD) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Surfactants - Anionic																

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Pentafluoropionamide	354-76-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Heptafluorobutyramide	662-50-0		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Perfluorooctanamide	423-54-1		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Nonafluoropentanamide	13485-61-5		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Perfluoropentanamide	355-61-7		No alert found	No alert found	No alert found	Acylation; Acylation >> P450 Mediated Activation to Acyl Halides; Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Perfluorooctanedioic diamide	3492-23-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Octafluorodipionamide	355-66-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																


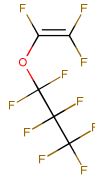
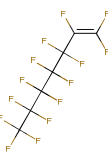
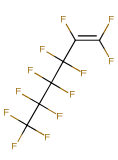
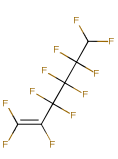
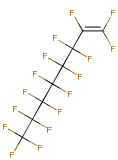
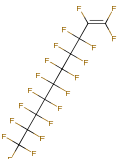
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 変異試験	遺伝毒性 in vitro マウスリンフォーム試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷試験	遺伝毒性 in vivo 変異試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メット試験	In vivo 突然変異	発がん性	
N-Methylperfluorooctanamide	89932-74-1		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Haloacetamide; Organic amide and thioamide; Perfluorocarbon derivatives																
Perfluoropentane sulfonic acid	2706-91-4		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																
Perfluorononane sulfonic acid	68259-12-1		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																
Perfluorodecane sulfonic acid	335-77-3		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																
Perfluoroundecane sulfonic acid	749786-16-1		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																
Perfluorododecane sulfonic acid	79780-39-5		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																
Perfluorotridecane sulfonic acid	791563-89-8		No alert found	No alert found	AN2, AN2 >> Schiff base formation by aldehyde formed after metabolic activation; AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives; Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives; SN2, SN2 >> Acylation involving a leaving group after metabolic activation; SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation; SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Sulfonic acid; Surfactants - Anionic																

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追加 Ammonium perfluorooctanesulfonate	29081-56-9		No alert found	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																	
追加 Perfluorononanesulfonate	474511-07-4		No alert found	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonic acid;Surfactants - Anionic																	
1H,1H-Perfluoropropylamine	422-03-7		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																	
1H,1H-Heptafluorobutylamine	374-99-2		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																	
1H,1H-Perfluoroheptylamine	423-49-4		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																	
1H,1H-Perfluorooctylamine	307-29-9		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																	
1H,1H-Perfluorononylamine	355-47-5		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																	

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 復帰突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
1H,1H-Perfluorohexylamine	355-34-0		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																
1H,1H-Perfluoropentylamine	355-27-1		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																
1H,1H,2H-Perfluorocyclopentane	15290-77-4		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Halogenated Cycloalkane Type Compounds	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives	TA1535, TA1537, TA98,TA100, WP2 (±S9) Negative	human lymphocytes (±S9) Positive														
Perfluoro-1,2-dimethylcyclohexane	306-98-9		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives	TA1535, TA1537,TA98,TA100, WP2 (±S9) Negative	Chinese Hamster Lung Cells (±S9) Negative														
Perfluoro-1,3-dimethylcyclohexane	335-27-3		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives	TA1535,TA1537,TA98,TA100,WP2 (±S9) Negative	CHO (±S9) Negative														
Perfluoro-1,2-dimethylcyclobutane	2994-71-0		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives																
Perfluoromethylcyclohexane	355-02-2		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives																

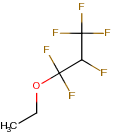
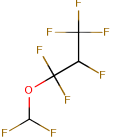
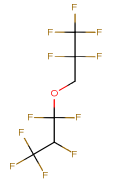
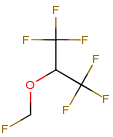
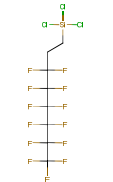
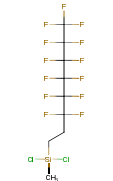
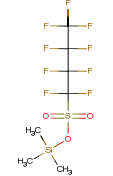
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成	In vitro 糖胎形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluoromethylcyclopentane	1805-22-7		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives																
Perfluoro-1,3,5-trimethylcyclohexane	374-78-5		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Cycloalkane;Perfluorocarbon derivatives																
2(Perfluoro-2-propyl)ethanol	9099-87-4			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
2-Perfluoropropyl-2-propanol	355-22-6			No alert found	No alert found	No alert found	Alpha- and beta-Haloether (Reactive Functional Groups)	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
3(Perfluoro-2-butyl)propanol	239463-96-8			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
3-(Perfluoroisopropyl)propanol	29819-73-6			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
Hexafluoro-2-methyl-2-propanol	1515-14-6			No alert found	No alert found	No alert found	Alpha- and beta-Haloether (Reactive Functional Groups)	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																

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Nonafluoro-tert-butanol	2378-02-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																	
2-(4H-Perfluorobutyl)-2-propanol	2673-15-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																	
Methyl heptafluoropropylketone	355-17-9		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																	
Methyl perfluoropentylketone	2708-07-8		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																	
Methyl 4H-perfluorobutylketone	93449-49-1		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																	
4-(Perfluorobutyl)-2-butanone	140834-64-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																	
Methyl perfluoroethylketone	374-41-4		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																	

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Ethyl perfluoropentyl ketone	383177-55-7		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ketone; Perfluorocarbon derivatives																
Perfluoropropyl trifluorovinyl ether	1623-05-8		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives	TA97,TA98, TA100,TA1535, WP2 umA(±S9)Negative/Positive(NBIS)	human lymphocyte (±S9)Negative														
Perfluorooct-1-ene	355-63-5		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives																
Perfluorooct-1-ene	755-25-9		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives																
6H-Perfluorooct-1-ene	1767-94-8		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	Acylation:Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives																
Perfluorooct-1-ene	559-14-8		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives																
Perfluorodec-1-ene	35328-43-9		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetraachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Unsaturated perhalogenated carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro Hprt試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
2H-Perfluoro-2-propanol	920-66-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives	TA1535, TA1537, TA1538, TA97, TA98, TA100, WP2 UvrA (± S9) Negative															
1H,1H,3H-Perfluorobutanol	382-31-0		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives																
2-Iodo-1H,1H,2H,3H,3H-perfluorodecan-1-ol	16083-64-0		Aliphatic halogens (Genotox);Stru clural alert for genotoxic carcinogenicity	Radical,Radical >> ROS formation after GSH depletion (indirect);Radical >> ROS formation after GSH depletion (indirect) >> Halalcohols;SN2;SN2 >> Alkylation by epoxide metabolically formed after E2 reaction;SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Halalcohols	Radical,Radical >> ROS formation after GSH depletion (indirect);Radical >> ROS formation after GSH depletion (indirect) >> Halalcohols;SN2;SN2 >> Alkylation by epoxide metabolically formed after E2 reaction;SN2 >> Alkylation by epoxide metabolically formed after E2 reaction >> Halalcohols	SN2;SN2 >> SN2 at an sp3 Carbon atom;SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Alpha- and beta-Haloether Reactive Functional Groups	Aliphatic halogens	Aliphatic halogen	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives																
1-Perfluoropropylethanol	375-14-4		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives																
1-Pentafluoroethylethanol	374-40-3		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives																
1H,1H,1H,2H-Perfluoro-2-heptanol	914637-05-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol,Alkane, branched with secondary carbon,Alkyl halide,Perfluorocarbon derivatives																
(Perfluorobutyl)ethene	19430-93-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	No alert found	No alert found	Alkene moiety,Alkyl halide,Perfluorocarbon derivatives	TA1535, TA1537, TA98,TA100, WP2 (±S9) Negative	Chinese hamster Ovary (CHO)(±S9) Negative	mouse lymphoma L5178Y cells(±S9) Negative													

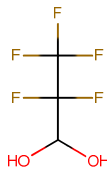




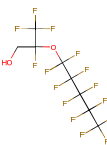
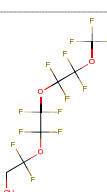
名称	OASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復雑突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コマンド試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRRT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コマンド試験	In vivo 突然変異	発がん性
1,6-Divinylperfluorohexane	1800-91-5		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Perfluorocarbon derivatives	TA1535, TA1537,TA98,TA100, TA102, WP2uvrA (±S9) Negative	peripheral human lymphocytes (±S9) Negative	mouse lymphoma L5178Y (±S9) Negative													
1H,1H,2H-Perfluoro-1-decene	21852-58-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Perfluorocarbon derivatives																
1,4-Divinylperfluorobutane	678-65-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Perfluorocarbon derivatives																
(Perfluoroheptyl)ethene	25431-45-2		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Perfluorocarbon derivatives																
1,8-Divinylperfluorooctane	35192-44-0		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Perfluorocarbon derivatives																
Hexafluoroisopropyl methyl ether	13171-18-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkanes, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives	TA1535, TA100; all common strains used in Ames assay (±S9) Negative															
(2H-Perfluoropropyl)(1H,1H-perfluoroethyl) ether	993-95-3		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkanes, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives																

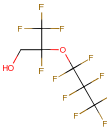
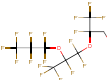
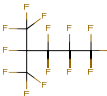
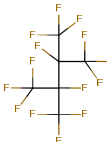
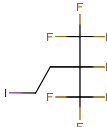
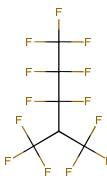
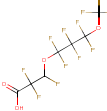
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA 鎖切断試験	遺伝毒性 in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性
Ethyl 2H-perfluoropropyl ether	380-34-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
Difluoromethyl 2H-perfluoropropyl ether	56860-65-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
1H,1H,2H-Perfluorodipropyl ether	1000-28-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
Sevoflurane	28523-86-6		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
Trichloro(perfluorohexyl)ethane	78560-45-9		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Silane	TA1535, TA1537, TA98,TA100, TA102 (±S8) Negative	Chinese hamster lung fibroblasts (V79) (±S8) Negative	mouse lymphoma L5178Y cells (±S8) Negative												
Dichloromethyl(perfluorohexyl)ethane	73609-36-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Silane															
Trimethylsilyl perfluorobutanesulfonate	68734-62-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Silane															

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性: vitro 復帰突然変異試験	遺伝毒性: vitro 染色体異常試験	遺伝毒性: in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性: vitro 小核試験	遺伝毒性: vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性: vivo 小核試験	遺伝毒性: vivo DNA損傷	遺伝毒性: in vivo 体異常試験	遺伝毒性: in vivo 染色体DNA合成試験	遺伝毒性: in vivo 不定期DNA合成/メット試験	In vivo 突然変異	発がん性
2-(Perfluorooctyl)ethyl(dimethyl)chlorosilane	74612-30-9		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Silane																
(Heptafluoropropyl)trimethylsilane	3834-42-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Silane																
2H-Perfluorobutyric acid	564-10-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
3-(Perfluoro-2-butyl)propanoic acid	239463-95-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Perfluoro-3,7-dimethyloctanoic acid	172155-07-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether;Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
2(2H-Perfluoro-2-propyl)acetic acid	17327-33-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
4,4-bis(Trifluoroethyl)-4-fluoropropionic acid	243139-62-0		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotoxa and nongenotoxa) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーム試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	In vitro HPR1試験	In vitro 定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo突然変異	発がん性
1H,1H,3H-Perfluoropropyl triflate	6401-02-1		Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid) (Genotox.)Structural alert for genotoxa carcinogenicity	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Not classified	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester																
3H,3H-Perfluoropropyl triflate	6401-00-9		Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid) (Genotox.)Structural alert for genotoxa carcinogenicity	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Not classified	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester																
2,2,2-Trifluoroethyl perfluorobutanesulfonate	79963-95-4		Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid) (Genotox.)Structural alert for genotoxa carcinogenicity	No alert found	No alert found	No alert found	Not classified	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester																
1H,1H-Heptafluorobutyl triflate	6401-01-0		Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid) (Genotox.)Structural alert for genotoxa carcinogenicity	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2,SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Not classified	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester																
1H,1H-Perfluorobutyl perfluorobutanesulfonate	883499-32-9		Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid) (Genotox.)Structural alert for genotoxa carcinogenicity	No alert found	No alert found	No alert found	Not classified	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl (C(S) or benzyl ester of sulphonate or phosphonic acid)	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester																
追加 1,1,2,2-pentafluoroethyl perfluorobutanesulfonate	354-87-0		No alert found	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives;SN2 >> SN2 at sulfur atom;SN2 >> SN2 at sulfur atom >> Sulfonate Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester	Positive(NBS)															
Perfluorobutanesulfonate fluoride	375-72-4		No alert found	No alert found	SN2,SN2 >> SN2 attack on sulfur atom;SN2 >> SN2 attack on sulfur atom >> Sulfonate Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonate ester	TA1535, TA1537, TA98, TA100, WP2uvrA, pKM101 (±59) Negative	human lymphocytes (±59) Negative														

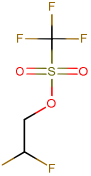
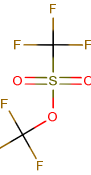
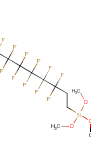
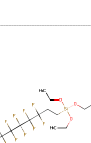

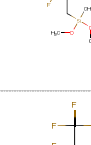
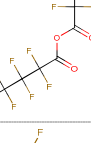
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by EIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 体質異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluorooctanesulfonyl fluoride	307-35-7		No alert found	No alert found	SN2,SN2 >> SN2 attack on sulfur atom;SN2 >> SN2 attack on sulfur atom >> Sulfonyl Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonyl halide	TA98,TA100 (±S9) Negative																
Perfluoro-1-butanesulfonyl chloride	2991-84-6		No alert found	No alert found	SN2,SN2 >> SN2 attack on sulfur atom;SN2 >> SN2 attack on sulfur atom >> Sulfonyl Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonyl halide																	
Perfluoro-1-octanesulfonyl chloride	423-60-9		No alert found	No alert found	SN2,SN2 >> SN2 attack on sulfur atom;SN2 >> SN2 attack on sulfur atom >> Sulfonyl Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Sulfonyl halide																	
1H,1H,8H,8H-Perfluorooctane-1,8-diol	90177-96-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Dihydroxy derivatives;Perfluorocarbon derivatives																	
Hexafluoroethylene glycol	376-90-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Dihydroxy derivatives;Perfluorocarbon derivatives																	
1H,1H,10H,10H-Perfluorodecane-1,10-diol	754-96-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Dihydroxy derivatives;Perfluorocarbon derivatives																	
1H,1H,6H,6H-Perfluoro-1,6-hexanediol	355-74-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Dihydroxy derivatives;Perfluorocarbon derivatives																	

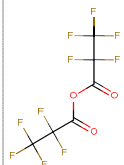



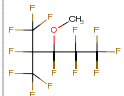
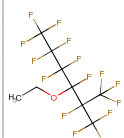
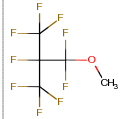
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常等試験	遺伝毒性 in vitro マウスリンフォーマ試験	in vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	in vitro HPRIT試験	in vitro 不 定期DNA合 成	in vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不足メット試験	in vitro 突然変異	発がん性
1H-Perfluoro- propanediol	422-63-9		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Dihydroxy derivatives;Per fluorocarbon derivatives																
Perfluorooctan esulfonamide	754-91-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluor ocarbon derivatives;Sul fonamide																
N- Ethylperfluoro octane sulfonamide	4151-50-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluor ocarbon derivatives;Sul fonamide																
N- Methylperfluor ooctanesulfona mide	31506-32-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluor ocarbon derivatives;Sul fonamide																
Perfluorohexan esulfonamide	41997-13-1		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluor ocarbon derivatives;Sul fonamide																
2,3,3'- Tetrafluoro-2- (perfluoropent oxy)propan-1- ol	76693-85-3		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	H ⁺ -acceptor- path3-H ⁺ - acceptor	Alcohol;Alkyl halide;Ether moiety;Perflu ocarbon derivatives																
1H,1H'- Perfluoro- 3,6,9- trioxadecan- 1-ol	147492-57-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	H ⁺ -acceptor- path3-H ⁺ - acceptor	Alcohol;Alkyl halide;Ether moiety;Perflu ocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性: vitro 復帰突然変異試験	遺伝毒性: vitro 染色体異常試験	遺伝毒性: in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性: vitro 小核試験	遺伝毒性: vitro DNA鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性: vivo 小核試験	遺伝毒性: vivo DNA損傷	遺伝毒性: in vivo 染色体異常試験	遺伝毒性: in vivo 染色体DNA合成試験	遺伝毒性: in vivo コメット試験	In vivo 突然変異	発がん性
2-(Perfluoropropoxy)-1H,1H-perfluoropropanol	26537-88-2		No alert found	No alert found	No alert found	SN1:SN1 >> Carbenium Ion Formation SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
1H,1H-Perfluoro-2,5-dimethyl-3,6-dioxanonan-1-ol	14548-74-4		No alert found	No alert found	No alert found	SN1:SN1 >> Carbenium Ion Formation SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
Perfluoroisobutane	355-04-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives	TA1535, TA1537, TA98,TA100, WP2 (not specified) Negative	Chinese hamster Ovary (CHO) (±S9) Negative														
Perfluoro-2,3-dimethylbutane	354-96-1		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
2-(2-Iodoethyl)perfluoropropane	99324-96-6		Aliphatic halogens (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	SN2:SN2 >> SN2 at an sp3 Carbon atom SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	Aliphatic halogens	Aliphatic halogen	Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
2H-Perfluoro(2-methylpentane)	30320-28-6		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives																
4,8-Dioxo-3H-perfluorooxanoic acid	919005-14-4 958445-44-8		No alert found	No alert found	No alert found	SN1:SN1 >> Carbenium Ion Formation SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Carboxylic acid;Ether moiety;Perfluorocarbon derivatives	TA1535, TA1537, TA98,TA100, WP2,uvrA(±S9) Negative	ヒトリンパ球(±S9) False Positive		V79(±S9) Negative		NMR/IR/マウス骨髄(経口) Negative	Wistarラット骨髄(経口) Negative								

[illegible]

名称	QASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複発突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
1H,1H-Heptafluorobutyl epoxide	1765-92-0		Epoxides and aziridines (Genotox); Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Direct Acting Epoxides and related;SN2 >> Direct Acting Epoxides and related >> Epoxides	Epoxide Reactive Functional Groups	Epoxides and aziridines	Epoxides and aziridines	Alkyl halide;Epoxide; Perfluorocarbon derivatives;Saturated heterocyclic fragment																
3-(Perfluorohexyl)-1,2-epoxypropane	35565-52-5		Epoxides and aziridines (Genotox); Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Direct Acting Epoxides and related;SN2 >> Direct Acting Epoxides and related >> Epoxides	Epoxide Reactive Functional Groups	Epoxides and aziridines	Epoxides and aziridines	Alkyl halide;Epoxide; Perfluorocarbon derivatives;Saturated heterocyclic fragment																
3-(Perfluorooctyl)-1,2-epoxypropane	35565-53-6		Epoxides and aziridines (Genotox); Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Direct Acting Epoxides and related;SN2 >> Direct Acting Epoxides and related >> Epoxides	Epoxide Reactive Functional Groups	Epoxides and aziridines	Epoxides and aziridines	Alkyl halide;Epoxide; Perfluorocarbon derivatives;Saturated heterocyclic fragment																
3-(Perfluorobutyl)-1,2-diol	125070-38-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkane, branched with secondary carbon;Alkyl halide;Dihydroxyl derivatives;Perfluorocarbon derivatives																
3-(Perfluoropropyl)-1,2-propanediol	1992-91-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkane, branched with secondary carbon;Alkyl halide;Dihydroxyl derivatives;Perfluorocarbon derivatives																
1-(Perfluorooctyl)propane-2,3-diol	94159-84-9		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkane, branched with secondary carbon;Alkyl halide;Dihydroxyl derivatives;Perfluorocarbon derivatives																
2,2,2-Trifluoroethyl triflate	6220-25-1		Alkyl (O-G) or benzyl ester of sulphonic or phosphonic acid (Genotox); Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Not classified	Alkyl (O-G) or benzyl ester of sulphonic or phosphonic acid	Alkyl (O-G) or benzyl ester of sulphonic or phosphonic acid	Alkyl halide;Sulfonate ester	TA98,TA1537, WP2 UvrA(±S9) Negative, TA1535(±S9) Positive, TA100 (+S9) Negative, (-S9) Positive // Positive(NBHS)															


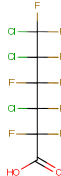
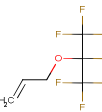
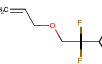
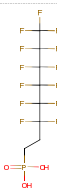

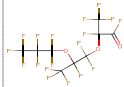
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA 鎖切断試験	in vitro HPRIT試験	in vitro 定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 vivo 小試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メット試験	in vivo 突然変異	発がん性
2,2-Difluoroethyl triflate	74427-22-8		Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid (Genotox)) Structural alert for genotoxic carcinogenicity	Radical/Radical >> ROS formation after GSH depletion/Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical/Radical >> ROS formation after GSH depletion/Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Not classified	Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid	Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid	Alkyl halide;Sulfonate ester														
Trifluoromethyl trifluoromethanesulfonate	35827-05-6		Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid (Genotox)) Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Not classified	Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid	Alkyl (C(S) or benzyl ester of sulphonic or phosphonic acid	Alkyl halide;Sulfonate ester														
[2-(Perfluorohexyl)ethyl]trimethylsilane	85857-16-5		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkoxyalkane;Alkyl halide;Perfluorocarbon derivatives;Silane	TA1535, TA1537, TA98, TA100, TA102 (±S8) Negative													
Triethoxy(perfluorohexyl)ethylsilane	51851-37-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkoxyalkane;Alkyl halide;Perfluorocarbon derivatives;Silane	TA1535, TA1537, TA98, TA100, TA102 (±S8) Negative	Chinese hamster lung fibroblast V79 (±S8) Negative	mouse lymphoma L5178Y fibroblast V79 (±S8) Negative											
Dimethoxy(perfluorohexyl)ethylsilane	85857-17-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkoxyalkane;Alkyl halide;Perfluorocarbon derivatives;Silane														
Perfluorobutanedioic anhydride	336-59-4		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H+acceptor-path3-H+acceptor	Acid anhydride;Alkyl halide;Perfluorocarbon derivatives														
2H-Perfluoropropanoic anhydride	337-63-7		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Not classified	No alert found	H+acceptor-path3-H+acceptor	Acid anhydride;Alkyl halide;Perfluorocarbon derivatives														

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Pentafluoropropionic anhydride	356-42-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Acid anhydride; Alkyl halide; Perfluorocarbon derivatives																
2-(Perfluorooctyl)ethanethiol	34143-74-3		No alert found	No alert found	Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Thiols	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Thiol																
2-(Perfluorohexyl)ethanethiol	34451-26-8		No alert found	No alert found	Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Thiols	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Thiol																
2-(Perfluorobutyl)ethanethiol	34451-25-7		No alert found	No alert found	Radical; Radical >> Radical mechanism via ROS formation (indirect); Radical >> Radical mechanism via ROS formation (indirect) >> Thiols	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Perfluorocarbon derivatives; Thiol																
3-Methoxyperfluorooctyl 2-methylpentanoate	132182-92-4		Structural alert for nongenotoxic carcinogenicity: Substituted n-alkylcarboxylic acids (Nongenotox)	No alert found	No alert found	SN1; SN1 >> Carbenium Ion Formation; SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon; Alkyl halide; Ether moiety; Perfluorocarbon derivatives	TA1535, TA1537, TA98, TA100, WP2 (±S9) Negative	peripheral human lymphocytes (±S9) Negative	mouse lymphoma L5178Y (±S9) Negative													
3-Ethoxyperfluorooctyl 2-methylhexanoate	297302-93-9		Structural alert for nongenotoxic carcinogenicity: Substituted n-alkylcarboxylic acids (Nongenotox)	No alert found	No alert found	SN1; SN1 >> Carbenium Ion Formation; SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon; Alkyl halide; Ether moiety; Perfluorocarbon derivatives	TA1535, TA1537, TA98, TA100, WP2 (±S9) Negative	CHL/IU (±S9) Negative	lymphoma L5178Y cells (±S9) Negative													
Perfluorooctobutyl methyl ether	163702-08-7		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon; Alkyl halide; Ether moiety; Perfluorocarbon derivatives																

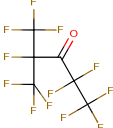
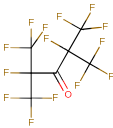
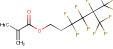
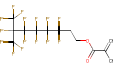
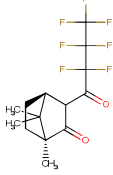
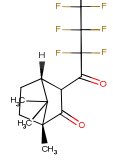
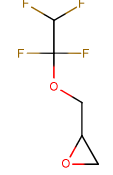
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by IIS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by IIS	In vivo mutagenicity (Micronucleus) alerts by IIS	Organic functional groups	遺伝毒性 in vitro 復帰突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Pentafluoropyrimidine	422-62-8		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Amidine; Perfluorocarbon derivatives															
Perfluorobutylamine	375-19-9		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Amidine; Perfluorocarbon derivatives															
Perfluorooctanamine	307-31-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Amidine; Perfluorocarbon derivatives															
tris(Trifluoroethoxy)methane	58244-27-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety															
Fluorethyl	333-36-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety															
1,1,2-Trifluoro-1-methoxy-2-(trifluoromethoxy)ethane	996-56-5		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Ether moiety															
2H,3H-Perfluoropentane	138495-42-8		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Perfluorocarbon derivatives	TA1535, TA97, TA98, TA100, WP2 uvrA pKM101 (±S0) Negative	human lymphocytes (±S0) Negative	mouse lymphoma L5178Y (±S0) Negative												

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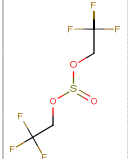
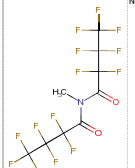
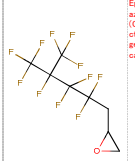
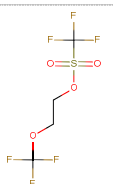
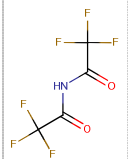
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 変異試験	遺伝毒性 in vitro 変異試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA 損傷試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小腸試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 体変異試験	遺伝毒性 in vivo 体変異試験	遺伝毒性 in vivo DNA合成試験	遺伝毒性 in vivo 不定期DNA合成試験	in vivo 突然変異	発がん性
3H,3H-Perfluoro-2,4-hexanedione	20825-07-4		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alkyl halide;Ketone;Perfluorocarbon derivatives																
2,2-bis(trifluoromethyl)-2-hydroxyacetic acid	662-22-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
3,3-Bis(trifluoromethyl)-3-hydroxypropionic acid	1547-36-0		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
1H,1H,1H,1H-Perfluorotetraethylene glycol	330562-44-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alcohol;Alkyl halide;Dihydroxyl derivatives;Ether moiety;Perfluorocarbon derivatives																
1H,1H,1H,1H-Perfluoro-3,6-dioxatane-1,8-diol	129301-42-4		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alcohol;Alkyl halide;Dihydroxyl derivatives;Ether moiety;Perfluorocarbon derivatives																
N,N-dimethyl-2H-perfluoroethanamine	1550-50-1		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;SN1;SN1 >> Imine;Imine Formation;SN1 >> Aliphatic tertiary amines	Alpha-Haloalkylamine Reactive Functional Groups;Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, tertiary;Alkyl halide;Amine, tertiary;Perfluorocarbon derivatives																
Perfluoramine	338-63-0		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;SN1;SN1 >> Imine;Imine Formation;SN1 >> Aliphatic tertiary amines	Alpha-Haloalkylamine Reactive Functional Groups;Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, tertiary;Alkyl halide;Amine, tertiary;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常等試験	遺伝毒性 in vitro マウスリンフローマ試験	in vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常等試験	遺伝毒性 in vivo DNA合成試験	遺伝毒性 in vivo 不足メット試験	in vitro 突然変異	発がん性
3,5,7,8-Tetrachloroperfluorooctanoic acid	2923-68-4		No alert found	No alert found	SN2;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihaloalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid;Perhalogenated carbon derivatives	TA1535, TA1537, TA1538, TA98, TA100(±S9) Negative															
3,5,6-Trichloroperfluorooctanoic acid	2106-54-9		No alert found	No alert found	SN2;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihaloalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid;Perhalogenated carbon derivatives	TA1535, TA1537, TA1538, TA98, TA100(±S9) Negative															
Alkyl perfluoroisopropyl ether	15242-17-8		No alert found	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
3-(2,2,3,3-Tetrafluoropropoxy)prop-1-ene	681-68-5		No alert found	No alert found	No alert found	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkyl halide;Ether moiety;Perfluorocarbon derivatives																
2-(Perfluorooctylethyl)phosphonic acid	252237-40-4		No alert found	No alert found	No alert found	No alert found	Organophosphorus Type Compounds	No alert found	No alert found	(Thio)Phosphonic acid derivatives;Alkyl halide;Perfluorocarbon derivatives;Phosphonic acid	[No test] TA1535, TA1537, TA98, TA100, WP2umA(±S9) Negative]						[No test] V79(±S9) Negative]									
((Perfluorooctylethyl)phosphonic acid	80220-63-9		No alert found	No alert found	No alert found	No alert found	Organophosphorus Type Compounds	No alert found	No alert found	(Thio)Phosphonic acid derivatives;Alkyl halide;Perfluorocarbon derivatives;Phosphonic acid																
Hexafluoroisopropene oxide	2641-34-1		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide;SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Acyl and Benzoyl Type Compounds;Alpha- and beta-Haloether Reactive Functional Groups	Acyl halides	Acyl halides;H-acceptor;H+-acceptor	Acyl halide;Alkyl halide;Ether moiety;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複発突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRTT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Perfluoro(2-methyl-3-oxahepta-1-yl) fluoride	2062-98-8		Acyl halides (Genotox); Structural alert for genotoxic carcinogenicity	No alert found	SN2, SN2 >> Direct acylation involving a leaving group; SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation; Acylation >> Direct Addition of an Acyl Halide; Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds; Alpha and beta-Haloether Reactive Functional Groups	Acyl halides	Acyl halides; H-acceptor-path3-H-acceptor	Acyl halide; Alkyl halide; Ether moiety; Perfluorocarbon derivatives																
4H,4H-Perfluoro-6,6-dimethylheptane-3,5-dione	2145-68-8		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide; Diketone; Ketone; Perfluorocarbon derivatives; tert-Butyl																
(Heptafluorobutyl)bis(alkyl) methane	17587-22-3		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide; Diketone; Ketone; Perfluorocarbon derivatives; tert-Butyl																
9-Chloro-perfluorononanoic acid	865-79-2		Perfluorooctanoic acid (PFOA) (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide; Carboxylic acid; Perfluorocarbon derivatives; Perhalogenated carbon derivatives																
5-Bromo-4,4,5,5-tetrafluoropentanoic acid	23443-22-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide; Carboxylic acid; Perfluorocarbon derivatives; Perhalogenated carbon derivatives																
Methyl perfluoro-3,6-dioxahexanoate	39187-41-2		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide; Carboxylic acid; Ester; Ether moiety; Perfluorocarbon derivatives																
Methyl perfluoro-2-propoxypropanoate	13140-34-6		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide; Carboxylic acid; Ester; Ether moiety; Perfluorocarbon derivatives																

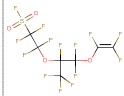
名称	QASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マット試験	遺伝毒性 in vitro コマンド試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	遺伝毒性 in vitro HPRIT試験	遺伝毒性 in vitro 定期DNA合成試験	遺伝毒性 in vitro 細胞質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 定期DNA合成試験	遺伝毒性 in vivo マット試験	in vivo 突然変異	発がん性
Perfluoro-2-methyl-3-pentanone	756-13-8		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Ketone;Perfluorocarbon derivatives	TA1535, TA1537, TA98,TA100, WP2 uvrA (±S8) Negative	Chinese hamster Ovary (CHO)Embryonic cells (±S9), mouse lymphoma L5178Y cells (±S8)Negative														
Bis(perfluorooctyloxy)ketone	813-44-5		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Ketone;Perfluorocarbon derivatives																
2-(Perfluoro-3-methylbutyl)ethyl methacrylate	85195-44-0		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
(Perfluoro-5-methylhexyl)ethyl 2-methylprop-2-enoate	50836-66-3		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
(1S,4S)-3-(Heptafluorobutyl)camphor	115224-00-5		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	Alkyl halide;Bicyclopentane;Bridged ring carbocycles;Cycloalkane;Cycloketone;Diastereone;Ketone;Perfluorocarbon derivatives;Terpenes																
(1R,4R)-3-(Heptafluorobutyl)camphor	51800-99-8		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	Alkyl halide;Bicyclopentane;Bridged ring carbocycles;Cycloalkane;Cycloketone;Diastereone;Ketone;Perfluorocarbon derivatives;Terpenes																
(2H-Perfluoroethoxy)methylsiloxane	85567-21-1		Epoxides and aziridines (Genotox);Structural alert for genotoxic carcinogenicity	Radical;Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiiranes and Oxetanes;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical;Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiiranes and Oxetanes;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;SN2;SN2 >> Direct Acting Epoxides and related;SN2 >> Direct Acting Epoxides and related >> Epoxides	Alpha- and beta-Haloether Reactive Functional Groups;Epoxide Reactive Functional Groups	Epoxides and aziridines	Epoxides and aziridines;H+acceptor-path3-H+acceptor	Alkyl halide;Epoxide;Ether moiety;Perfluorocarbon derivatives;Saturated heterocyclic fragment																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification (Ames test)	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーム試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メット試験	In vivo突然変異	発がん性
(2,2,3,3-Tetrafluoropropyl)methyl oxirane	19932-26-4		Epoxides and aziridines (Genotox);Structural alert for genotoxic carcinogenicity	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiranes and Oxetanes	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;SN2;SN2 >> Direct Acting Epoxides and related;SN2 >> Direct Acting Epoxides and related >> Epoxides	Alpha- and beta-Haloether Reactive Functional Groups;Epoxide and aziridines	Epoxides and aziridines	Epoxides and aziridines;H-acceptor-path3-H-acceptor	Alkyl halide;Epoxide; Ether moiety;Perfluorocarbon derivatives;Saturated heterocyclic fragment																
N-Ethyl-N-(2-hydroxyethyl)perfluorooctane sulfonamide	1691-99-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkyl halide;Perfluorocarbon derivatives;Sulfonamide																
N-Methyl-N-(2-hydroxyethyl)perfluorooctane sulfonamide	24448-09-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alcohol;Alkyl halide;Perfluorocarbon derivatives;Sulfonamide																
2-(Perfluorooctyl)ethyl dihydrogen phosphate	57678-03-2		No alert found	No alert found	SN2;SN2 >> Alkylation;SN2 >> Alkylation >> Alkylphosphates, Alkylthiophosphates and Alkylphosphonates	No alert found	Organophosphorus Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Phosphate ester																
6:2 Fluorotelomer phosphate monoester	57678-01-0		No alert found	No alert found	SN2;SN2 >> Alkylation;SN2 >> Alkylation >> Alkylphosphates, Alkylthiophosphates and Alkylphosphonates	No alert found	Organophosphorus Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Phosphate ester																
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid	756426-58-1		No alert found	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Ether moiety;Perfluorocarbon derivatives;Perhalogenated carbon derivatives;Sulfonic acid																
11-Chlorooctafluoro-3-oxaundecane-1-sulfonic acid	83329-89-9		No alert found	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Ether moiety;Perfluorocarbon derivatives;Perhalogenated carbon derivatives;Sulfonic acid																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフローマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA 鎖切断試験	遺伝毒性 in vitro Hprt試験	遺伝毒性 in vitro 不定期DNA合成試験	遺伝毒性 in vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo突然変異	発がん性	
追加	N-ethyl perfluorooctanesulfonamideacetic acid		No alert found	No alert found	AN2:AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives:Radical:Radical >> Radical mechanism via ROS formation (indirect):Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives:SN2:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Sulfonamide																
追加	N-methyl perfluorooctanesulfonamideacetic acid		No alert found	No alert found	AN2:AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives:Radical:Radical >> Radical mechanism via ROS formation (indirect):Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives:SN2:SN2 >> Acylation involving a leaving group after metabolic activation:SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation:SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide:Carboxylic acid:Perfluorocarbon derivatives:Sulfonamide																
	Bis(2,2,2-trifluoroethyl)sulfite		No alert found	SN2:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Not classified	No alert found	No alert found	Alkyl halide:Sulfite ester																
	N-Methyl-bis-heptafluorobutyramide		No alert found	No alert found	No alert found	SN1:SN1 >> Iminium Ion Formation:SN1 >> Iminium Ion Formation >> Aliphatic tertiary amines	Not classified	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide:Haloacetamide:Imide:Perfluorocarbon derivatives																
	3-(Perfluoro-3-methylbutyl)-1,2-propenoxide		Epoxides and aziridines (Genotox):Structural alert for genotoxic carcinogenicity	SN2:SN2 >> Alkylation, direct acting epoxides and related:SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiiranes and Oxetanes	SN2:SN2 >> Alkylation, direct acting epoxides and related:SN2 >> Alkylation, direct acting epoxides and related >> Epoxides, Aziridines, Thiiranes and Oxetanes	SN2:SN2 >> Direct Acting Epoxides and related:SN2 >> Direct Acting Epoxides and related >> Epoxides	Epoxide Reactive Functional Groups	Epoxides and aziridines	Epoxides and aziridines	Alkane, branched with tertiary carbon:Alkyl halide:Epoxide:Perfluorocarbon derivatives:Set of heterocyclic fragment																
	2-(Trifluoromethoxy)ethyl trifluoromethanesulfonate		No alert found	SN2:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom:SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide:Ether moiety:Sulfonate ester																
	Perfluorodiacetamide		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide:Ether moiety:Sulfonate ester																



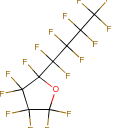
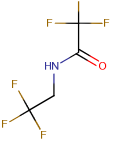
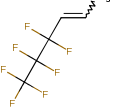
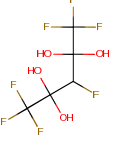
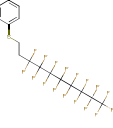
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常等試験	遺伝毒性 in vitro マウスリンフローマ試験	in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	in vitro HPRT試験	in vitro 不定期DNA合成	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常等試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vitro 突然変異	発がん性
1H,2H-Hexafluorocyclopentene	1005-73-8		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Halogenated Cycloalkane Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Cycloalkene moiety;Perfluorocarbon derivatives;Unsaturated carbocyclic fragment																
Hexafluorocyclopentyl acrylate	2160-89-6			No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes;Michael addition >> Polarised Alkenes;Michael addition >> Alpha, beta-unsaturated esters	Acrylate	No alert found	Acrylate;Alkanes, branched with secondary carbon;Alkene moiety;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives																
追加 sodium hydrogen(per)fluorohexylphosphonate	1189052-95-6			No alert found	No alert found	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Organophosphorus Type Compounds	No alert found	No alert found	Alkyl halide;Perfluorocarbon derivatives;Phosphonic acid	TA1535, TA1537, TA98, TA100, WP2uvrA(±S9) Negative				V79(±S8) Negative										
2-Bromo-2-(Perfluorohexyl)ethene	51249-64-0		Monohaloalkene (Genotox);Structural alert for genotox carcinogenicity	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	Monohaloalkene	Monohaloalkene	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives																
N,N-Diethyl-2H-perfluoropropylamine	309-88-6			No alert found	No alert found	No alert found	Alpha-Haloalkylamine;Reactive Functional Groups;Nitrogen Mustards;Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, tertiary;Alkane, branched with secondary carbon;Alkyl halide;Amine, tertiary;Perfluorocarbon derivatives																
Ethyl pentafluoropropyl acetate	663-35-4			No alert found	No alert found	No alert found	Reactive Ketone;Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	Alkyl halide;Carboxylic acid ester;Ketone;Perfluorocarbon derivatives																
3,3-Bis(trifluoromethyl)-2-propenoic acid	1763-28-6			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Acrylic acids;Alkene moiety;Alkyl halide;Carboxylic acid;Unsaturated perhalogenated carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複発突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro DNA鎖切断試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	遺伝毒性 in vitro 細胞形質転換試験	遺伝毒性 vivo 小試験	遺伝毒性 vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性
(Perfluorooctyl)hexyl(methanol)	28788-68-3		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkyl halide;Cycloalkane;Perfluorocarbon derivatives															
Bis(2,2,2-trifluoroethyl)amine	407-01-2			No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, secondary;Alkyl halide;Amine, secondary															
2,2,2-Trifluoroethyl trifluoroacetate	407-38-5			No alert found	No alert found	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid ester															
Perfluoro(2-bromoethyl vinyl ether)	85737-06-0		Structural alert for nongenotox carcinogenicity;Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene (Nongenotox)	Radical;Radical >> ROS formation after GSH depletion >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical;Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives;Perfluorinated carbon derivatives;Unsaturated perhalogenated carbon derivatives															
2,4,6-Tris(pentafluoroethyl)-1,3,5-triazine	858-46-8			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Aryl;Perfluorocarbon derivatives;Triazine															
Hexafluoruron	86479-06-3			No alert found	Radical;Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Radical;Radical >> ROS formation after GSH depletion;Radical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane Derivatives;SN2;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes;SN1;SN1 >> Nitrenium Ion formation;SN1 >> Nitrenium Ion formation >> Aromatic phenylureas	Alpha- and beta- Haloether Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor															
1H,1H,7H-Perfluoroheptyl 4-methylbenzene sulfonate	424-16-8		Benzenesulfonic ethers, methylation (Nongenotox); Structural alert for nongenotox carcinogenicity	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	SN2;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Sulfonates and Sulfates	Acylation;Acylation >> P450 Mediated Activation to Acyl Halides;Acylation >> P450 Mediated Activation to Acyl Halides >> 1,1-Dihaloalkanes	Not classified	No alert found	No alert found	Alkyl (hetero)arenes;Alkyl halide;Alkyl-, alkenyl- and alkylnyl (hetero)arenes;Aryl;Perfluorocarbon derivatives;Sulfonate ester															

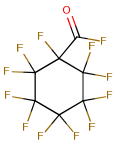
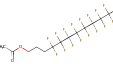
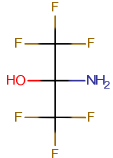
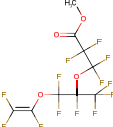
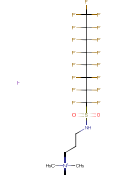
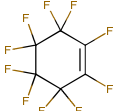
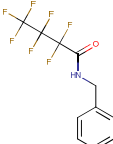
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複相突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	遺伝毒性 in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA鎖切断試験	in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性	
Perfluoro(4-methyl-3,6-dioxaoct-7-ene)sulfonyl fluoride	16090-14-5		Structural alert for nongenotoxic carcinogenicity (Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene (Nongenotox))	No alert found	SN2;SN2 >> SN2 attack on sulfur atom;SN2 >> SN2 attack on sulfur atom >> Sulfonyl Halides	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Ether moiety;Perfluorocarbon derivatives;Sulfonyl halide;Unsaturated perhalogenated carbon derivatives																	
Cyclohexafluoropropane-1,3-bis(sulfonyl)imide	84246-29-7		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Perfluorocarbon derivatives;Saturated heterocyclic fragment																	
2H-Perfluoroisopropyl 2-fluoroacrylate	74359-06-1		No alert found	AN2;AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> SN2 at sp3 and activated sp2 carbon atom >> Polarized Haloalkene Derivatives	AN2;AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> SN2 at sp3 and activated sp2 carbon atom >> Polarized Haloalkene Derivatives	AN2;AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Akylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> SN2 at sp3 and activated sp2 carbon atom >> Polarized Haloalkene Derivatives	Acrylate Reactive Functional Groups;Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkane, branched with secondary carbon;Alkene moiety;Alkenyl halide;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives																	
3H-Perfluoropentane-2,4-dione	77968-17-3		No alert found	SN2;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom >> Haloalkane Derivatives with Labile Halogen	SN2;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom >> Haloalkane Derivatives with Labile Halogen	SN2;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Akylation, nucleophilic substitution at sp3-carbon atom >> Haloalkane Derivatives with Labile Halogen	Reactive Ketone Reactive Functional Groups	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Diketone;Ketone																	
N-Methyl-N-trimethylsilylhexafluorobutyramide	53296-64-3		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Haloacetamide;Perfluorocarbon derivatives;Silane																	
(Perfluoroacyloxy)methyl prop-2-enoate	40677-94-9		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkyl halide;Carboxylic acid ester;Cycloalkane;Perfluorocarbon derivatives																	
3-(Perfluoroisopropyl)-2-propenoic acid	243139-64-2		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Acrylic acids;Alkane, branched with tertiary carbon;Alkene moiety;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																	

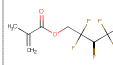
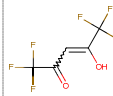
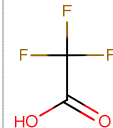
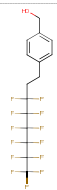
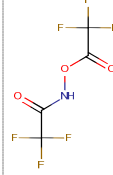
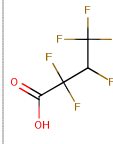
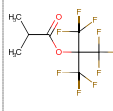
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複増突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
2-Allyloxyperfluorooctanesulfonyl fluoride	73806-13-0		No alert found	No alert found	SN2,SN2 >> SN2 attack on sulfur atom,SN2 >> SN2 attack on sulfur atom >> Sulfonyl Halides	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alkene moiety,Alkyl halide,Allyl Ether moiety,Perfluorocarbon derivatives,Sulfonyl halide																
Methyl 3-chloroperfluoropropanoate	127589-63-3		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide,Carboxylic acid ester,Perfluorocarbon derivatives,Perhalogenated carbon derivatives																
[(Heptafluoropropyl)sulfonyl]acetic acid	204057-69-2		No alert found	No alert found	No alert found	No alert found	Alpha-Haloether Reactive Functional Groups,Sulfur Mustard Reactive Functional Groups	No alert found	No alert found	Alkyl halide,Carboxylic acid,Perfluorocarbon derivatives,Sulfoxide																
4-[3-(Perfluorobutyl)-1-propenyl]benzyl alcohol	892154-51-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alcohol,Alkyl halide,Aryl,Benzyl,Ether moiety,Perfluorocarbon derivatives																
2-Vinyl(1-bromoperfluorooethane)	18599-22-9		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	No alert found	No alert found	Alkene moiety,Alkyl halide,Perfluorocarbon derivatives,Perhalogenated carbon derivatives																
2-Vinylperfluorooctane	239795-57-4		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	No alert found	No alert found	Alkene, branched with tertiary carbon,Alkene moiety,Alkyl halide,Perfluorocarbon derivatives																
Pentafluoroethyl fluorosulfate	67641-28-5		Structural alert for nongenotoxic carcinogenicity :Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkene moiety,Alkenyl halide,Alkyl halide,Unsaturated perhalogenated carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーム試験	In vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	In vitro HPRIT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
Bis(1H,1H-perfluoropropyl)amine	883498-76-8		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, secondary;Alkyl halide;Amine, secondary;Perfluorocarbon derivatives															
3-(Perfluorooctyl)triethylsulfonate	103229-89-6		No alert found	AN2:AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> Polarized Haloalkene Derivatives	AN2:AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation >> Thioacylation via nucleophilic addition after cysteine-mediated thioether formation >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> Polarized Haloalkene Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Acrylic acid;Alkane, branched with tertiary carbon;Alkene moiety;Alkyl halide;Carbonyl acid;Perfluorocarbon derivatives															
2H-Perfluorooctyl ether	59158-81-5		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkene moiety;Alkyl halide;Allyl ether moiety;Perfluorocarbon derivatives															
Hexafluoroacetone dihydrate	66922-83-6		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups;Not classified	No alert found	H-acceptor;path3-H-acceptor;No alert found	Alkyl halide;Diketone;Ketone;No functional group found															
Perfluorooctyl alcohol	918-21-8		Structural alert for nongenotoxic carcinogenicity;Substituted n-alkylcarboxylic acids (Nongenotox)	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor;path3-H-acceptor	Alcohol;Alkane, branched with tertiary carbon;Alkyl halide;Dihydroxy derivatives;Perfluorocarbon derivatives															
(Perfluoro-3-methylbutyl)-2-hydroxypropyl acrylate	16083-76-4		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarized Alkenes-Michael addition;Michael addition >> Polarized Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	H-acceptor;path3-H-acceptor	Acrylate;Alcohol;Alkane, branched with secondary carbon;Alkane, branched with tertiary carbon;Alkene moiety;Alkyl halide;Carbonyl acid ester;Perfluorocarbon derivatives															
Tris(2,2,2-trifluoroethyl) borate	659-18-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Borate ester															

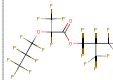
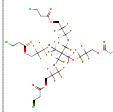
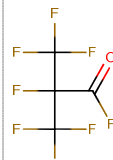
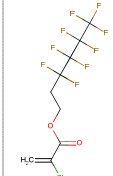

名称	QASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 <small>in vitro</small> 変異試験	遺伝毒性 <small>in vitro</small> 変異試験	遺伝毒性 <small>in vitro</small> マット試験	遺伝毒性 <small>in vitro</small> コマンド試験	遺伝毒性 <small>in vitro</small> DNA 損傷試験	遺伝毒性 <small>in vitro</small> HPRIT試験	遺伝毒性 <small>in vitro</small> 不定期DNA合成試験	遺伝毒性 <small>in vitro</small> 細胞質転換試験	遺伝毒性 <small>in vivo</small> 小試験	遺伝毒性 <small>in vivo</small> DNA損傷	遺伝毒性 <small>in vivo</small> 染色体異常試験	遺伝毒性 <small>in vivo</small> 不定期DNA合成試験	遺伝毒性 <small>in vivo</small> マット試験	遺伝毒性 <small>in vivo</small> 変異	発がん性
Perfluorooctanoic anhydride	699-30-9		No alert found	No alert found	No alert found	No alert found	Anhydride Type Compounds	No alert found	H-acceptor path3-H-acceptor/Oxalane	Acid anhydride;Alkyl halide;Oxalane;Perfluorocarbon derivatives															
1,1-bis(Trifluoromethyl)ethanol	63693-13-0		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor path3-H-acceptor	Alcohol;Alkane, branched with secondary carbon;Alkyl halide;Ether moiety;Perfluorocarbon derivatives															
Perfluoro-2-butyltetrahydrofuran	335-36-4		(Poly) Halogenated Cycloalkanes (Nongenotox). Structural alert for nongenotox carcinogenicity	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	Oxalane	Alkyl halide;Ether moiety;Oxalane;Perfluorocarbon derivatives;Saturated heterocyclic fragment															
2,2,2-Trifluoro-N-(2,2,2-trifluoroethyl)acetamide	407-37-4		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Haloacetamide;Organic amide and thioamide															
1-Propenylperfluoropropane	355-95-3		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkene moiety;Alkyl halide;Alkyl;Perfluorocarbon derivatives															
3H-Perfluoro-2,2,4,4-tetrahydroxypentane	77853-71-0		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alcohol;Alkane, branched with secondary carbon;Alkyl halide															
4-(1H,1H,2H,2H-Perfluorodecyl)thiophenol	142623-70-9		No alert found	No alert found	No alert found	No alert found	Phenol Type Compounds	No alert found	No alert found	Alkyl halide;Aryl;Perfluorocarbon derivatives;Phenol;Sulfide															

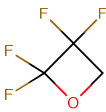
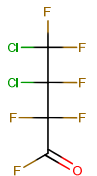

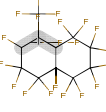
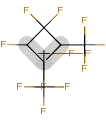
名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性: vitro 復帰突然変異試験	遺伝毒性: vitro 染色体異常試験	遺伝毒性: in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性: vitro 小核試験	遺伝毒性: vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成試験	In vitro 細胞形質転換試験	遺伝毒性: vivo 小核試験	遺伝毒性: vivo DNA損傷	遺伝毒性: in vivo 染色体異常試験	遺伝毒性: in vivo 不定期DNA合成試験	遺伝毒性: in vivo コメット試験	In vivo 突然変異	発がん性
2-Amino-2H-perfluoropropane	1619-92-7		No alert found	No alert found	No alert found	No alert found	Nitrogen Mustards Reactive Functional Groups	No alert found	No alert found	Aliphatic amine, primary;Alkane, branched with secondary carbon;Alkyl halide;Amine, primary;Perfluorocarbon derivatives																
Perfluoro(N-methylmorpholine)	382-28-5		(Poly) Halogenated Cycloalkanes (Nongenotox). Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups;Alpha-Haloalkylamine Reactive Functional Groups;Nitrogen Mustards Reactive Functional Groups	No alert found	H+acceptor-path3-H+ acceptor	Aliphatic amine, tertiary;Alkyl halide;Amine, tertiary;Ether moiety;Morpholine;Perfluorocarbon derivatives;Saturated heterocyclic fragment																
(Perfluorobutyl)-2-thenylmethane	559-94-4		No alert found	No alert found	No alert found	Michael addition;Michael addition >> P450 Mediated Activation of Heterocyclic Ring Systems;Michael addition >> P450 Mediated Activation of Heterocyclic Ring Systems >> Thiophenes-Michael addition;SN2;SN2 >> P450 Mediated Epoxidation;SN2 >> P450 Mediated Epoxidation >> Thiophenes; SN2	Reactive Ketone Reactive Functional Groups	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide;Aryl;Ketone;Ketone;Perfluorocarbon derivatives;Thiophene																
N-(3-(Dimethylamino)propyl)perfluorohexanesulfonamide	50598-28-2		No alert found	No alert found	No alert found	SN1;SN1 >> Iminium Ion Formation;SN1 >> Iminium Ion Formation >> Aliphatic tertiary amines	Not classified	No alert found	No alert found	Aliphatic amine, tertiary;Alkyl halide;Amine, tertiary;Perfluorocarbon derivatives;Sulfonamide																
(E)-Perfluoro(4-methyl-2-pentene)	3709-71-5		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkane moiety;Alkenyl halide;Alkyl halide;Perfluorocarbon derivatives																
Perfluoro-3,6-dimethyl-1,4-dioxan-2-one	7309-84-4		(Poly) Halogenated Cycloalkanes (Nongenotox). Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+ acceptor	Alkyl halide;Dioxane; Ether moiety;Lactones;Perfluorocarbon derivatives																
2-Chloro-perfluoro-2-methylpentane	67437-97-2		No alert found	No alert found	No alert found	No alert found	Halogenated Linear Aliphatic Hydrocarbons Type Compounds	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives;Perhalogenated carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	in vitro コメット試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	in vitro HprtT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	in vivo 突然変異	発がん性
Perfluorooctyl hexanecarboxyl fluoride	6588-63-2		(Poly) Halogenated Cycloalkanes (Nongenotox); Acyl halides (Genotox); Structural alerts for both genotox and nongenotox carcinogenicity	No alert found	SN2;SN2 >> Direct acylation involving a leaving group;SN2 >> Direct acylation involving a leaving group >> Acyl Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Cycloalkane;Perfluoroalkane;carbon derivatives																
(Perfluorooctyl)propyl acetate	150225-00-6			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Acetoxy;Alkyl halide;Carboxylic acid ester;Perfluoroalkane;carbon derivatives																
2-Aminoheptafluoropropan-2-ol	31253-34-6			No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups;Nitrogen Mustards;Reactive Functional Groups	No alert found	No alert found	Alcohol;Aliphatic amine, primary;Alkyl halide;Amine, primary;Perfluoroalkane;carbon derivatives																
Methyl perfluoro(3-(1-ethenyl)oxypropyl)-2-yl oxoxypropionate	63863-43-4		Structural alert for nongenotox carcinogenicity ;Trichloro (or fluoro) ethylene and Tetrachloro (or fluoro) ethylene (Nongenotox)	No alert found	No alert found	SN1;SN1 >> Carbenium Ion Formation;SN1 >> Carbenium Ion Formation >> Alpha halo ethers (including alpha halo thioethers)	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor;path3-H-acceptor	Alkene moiety;Alkenyl halide;Alkyl halide;Carboxylic acid ester;Ether moiety;Perfluoroalkane;carbon derivatives;Unsaturated perhalogenated carbon derivatives																
N-[(Perfluorooctylsulfonyl)amido]propyl-N,N,N-trimethylammonium iodide	1652-63-7			No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Perfluoroalkane;carbon derivatives;Quaternary ammonium salts;Sulfonamide																
Decafluorocyclohexene	355-75-9		(Poly) Halogenated Cycloalkanes (Nongenotox); Structural alert for nongenotox carcinogenicity	No alert found	No alert found	No alert found	Halogenated Cycloalkane Type Compounds	No alert found	No alert found	Alkene moiety;Alkenyl halide;Alkyl halide;Cycloalkene moiety;Perfluoroalkane;carbon derivatives;Unsaturated carbocyclic fragment																
N-(Phenylmethyl)perfluorobutanamide	560-02-1			No alert found	No alert found	No alert found	Michael addition;Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals;Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	Not classified	No alert found	Alkyl halide;Aryl;Benzyl;Haloacetamide;Organic amide and thioamide;Perfluoroalkane;carbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 復帰突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HprtT試験	In vitro 不定期DNA合成	In vitro 細胞形質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
1H,1H,3H-Perfluorobutyl 2-methylacrylate	36405-47-7		No alert found	No alert found	No alert found	Michael addition;Michael addition >> Polarised Alkenes-Michael addition;Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkene moiety;Alkyl halide;Allyl;Carboxylic acid ester;Methacrylate;Perfluorocarbon derivatives																
3H-Perfluoro-4-hydroxy-3-penten-2-one	1694-30-0		alpha,beta-unsaturated carbonyls (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups;Ketone Reactive Functional Groups	alpha,beta-unsaturated carbonyls	alpha,beta-unsaturated carbonyls;H-acceptor-path3-H-acceptor	Alkene moiety;Alkyl halide;Enol;Ketone																
Trifluoroacetic acid	76-05-1		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Carboxylic acid	TA1535,TA1537,TA98, TA100, TA102 (±S9) Negative	Human lymphocyte (±S9) Negative	lymphoma L5178Y cells(±S9) Negative													
4-((Perfluorohexylethyl)phenyl)methanol	356055-76-0		No alert found	No alert found	No alert found	Michael addition;Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals;Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	Not classified	No alert found	No alert found	Alcohol;Alkyl halide;Aryl;Benzyl;Perfluorocarbon derivatives																
N,O-Bis(trifluoroethyl)hydroxylamine	684-78-6		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H-acceptor-path3-H-acceptor	Alkyl halide;Haloacetamide																
3H-Perfluorobutanoic acid	379-90-8		No alert found	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkane, branched with secondary carbon;Alkyl halide;Carboxylic acid;Perfluorocarbon derivatives																
Perfluoro-tert-butyl isobutyrate	914637-43-7		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	No alert found	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid ester;Isopropyl;Perfluorocarbon derivatives																

名称	CASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for Ames, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronuclear) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 変異突然変異試験	遺伝毒性 in vitro 変異突然変異試験	遺伝毒性 in vitro コマンド試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	遺伝毒性 in vitro HPRIT試験	in vitro 不定期DNA合成試験	in vitro 細胞形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定メット試験	in vivo 突然変異	発がん性
3H,3H-Perfluoro-2-butanone	400-49-7		No alert found	No alert found	No alert found	No alert found	Reactive Ketone Reactive Functional Groups	No alert found	No alert found	Alkyl halideKetone															
Trifluoroacetic anhydride	407-25-0		No alert found	No alert found	No alert found	No alert found	Not classified	No alert found	H+acceptor-path3-H+acceptor	Acid anhydrideAlkyl halide															
5-Iodo-perfluoro-3-octanesulfonyle fluoride	66137-74-4		No alert found	RadicalRadical >> ROS formation after GSH depletionRadical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane DerivativesSN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane DerivativesSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugationSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane DerivativesSN2 >> SN2 attack on sulfur atomSN2 >> SN2 attack on sulfur atom >> Sulfonyle Halides	RadicalRadical >> ROS formation after GSH depletionRadical >> ROS formation after GSH depletion >> Geminal Polyhaloalkane DerivativesSN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane DerivativesSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugationSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane DerivativesSN2 >> SN2 attack on sulfur atomSN2 >> SN2 attack on sulfur atom >> Sulfonyle Halides	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	Alkyl halideEther moietyPerfluorocarbon derivativesPerhalogenated carbon derivativesSulfonyl halide															
追加 1H, 1H, 2H, 2H-perfluorooctyl acrylate	17527-29-6		No alert found	No alert found	AN2AN2 >> Schiff base formation by aldehyde formed after metabolic activationAN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane DerivativesRadicalRadical >> Radical mechanism via ROS formation (indirect)Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane DerivativesSN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane DerivativesSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugationSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Michael additionMichael addition >> Polarised Alkenes-Michael additionMichael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated esters	Acrylate Reactive Functional Groups	No alert found	No alert found	AcrylateAlkenic moietyAlkyl halideCarboxylic acid esterPerfluorocarbon derivatives	CHL/UL (±S8) Negative					V79 (±S8) Negative			CD-1マウス、経口、経鼻、経眼 Negative						
追加 Bis(2-hydroxyethyl)ammonium perfluorooctanesulfonic acid	70225-14-8		No alert found	No alert found	AN2AN2 >> Schiff base formation by aldehyde formed after metabolic activationAN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane DerivativesRadicalRadical >> Radical mechanism via ROS formation (indirect)Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane DerivativesSN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane DerivativesSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugationSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	H+acceptor-path3-H+acceptor	AlcoholAlkyl halideAmmonium saltDihydroxyl derivativesPerfluorocarbon derivativesSulfonic acidSurfactants - Anionic	ネズミマウス、経口、経鼻、経眼 Negative														
Lithium perfluorooctanesulfonate	29457-72-5		No alert found	No alert found	AN2AN2 >> Schiff base formation by aldehyde formed after metabolic activationAN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane DerivativesRadicalRadical >> Radical mechanism via ROS formation (indirect)Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane DerivativesSN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane DerivativesSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugationSN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Not classified	No alert found	No alert found	Alkyl halideLithium, organoPerfluorocarbon derivativesSulfonic acidSurfactants - Anionic															
Perfluoro(2-[5-methoxy-1,3-dioxolan-4-yl]oxy)acetic acid	1190931-41-9		(Poly) Halogenated Cycloalkanes (Nongenotox). Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H+acceptor-path3-H+acceptor	Alkyl halideCarboxylic acidDioxolane, Ether moietySaturated heterocyclic fragment															

名称	OASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncology Primary Classification	in vitro mutagenicity (Ames test) alerts by ISS	in vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 in vitro 複糖突然変異試験	遺伝毒性 in vitro 染色体異常試験	遺伝毒性 in vitro マウス試験	遺伝毒性 in vitro コマンド試験	遺伝毒性 in vitro 小核試験	遺伝毒性 in vitro DNA 鎖切断試験	遺伝毒性 in vitro HPRIT試験	遺伝毒性 in vitro 不定期DNA合成試験	遺伝毒性 in vitro 胎形質転換試験	遺伝毒性 in vivo 小核試験	遺伝毒性 in vivo DNA 損傷試験	遺伝毒性 in vivo 染色体異常試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コマンド試験	遺伝毒性 in vivo 突然変異	遺伝毒性 in vivo 発がん性	
追加 2-(3,4-dichloro-1,1,2,3,4,4-heptafluorobutoxy)-2,3,3,3-tetrafluoropropionic acid fluoride	NO_CAS		Acyl halides (Genotox)Structural alert for genotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical/Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihalooalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihalooalkanes;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds;Alpha- and beta-Haloether Reactive Functional Groups	Acyl halides	Acyl halides;H-acceptor-path;H-acceptor	Acyl halide;Alkyl halide;Ether moiety;Perfluorocarbon derivatives;Perhalogenated carbon derivatives	Positive(NBHS)																
追加 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propionic acid 2-trifluoromethylheptafluoropropyl ester	NO_CAS			No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical/Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	H-acceptor-path;H-acceptor	Alkane, branched with tertiary carbon;Alkyl halide;Carboxylic acid ester;Ether moiety;Perfluorocarbon derivatives	Positive(NBHS)																
追加 bis(3-chloropropyl)carbamate 3,3'-bis(2,3,3,3-tetrafluoropropoxy)bis(1,1,2,2-tetrafluoroethyl) 1,1,3,3-tetrafluoro-2,3,3,3-tetrafluoropropyl ester	NO_CAS		Aliphatic halogens (Genotox)Structural alert for genotoxic carcinogenicity	AN2,AN2 >> Schiff base formation for aldehydes;AN2 >> Schiff base formation for aldehydes >> Haloalkane Derivatives with Labile Halogen;SN2 >> Acylation involving a leaving group >> Haloalkane Derivatives with Labile Halogen;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Haloalkane Derivatives with Labile Halogen	AN2,AN2 >> Schiff base formation for aldehydes;AN2 >> Schiff base formation for aldehydes >> Haloalkane Derivatives with Labile Halogen;SN2 >> Acylation involving a leaving group >> Haloalkane Derivatives with Labile Halogen;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Haloalkane Derivatives with Labile Halogen	SN2;SN2 >> SN2 at an sp3 Carbon atom;SN2 >> SN2 at an sp3 Carbon atom >> Aliphatic halides	Alpha- and beta-Haloether Reactive Functional Groups	Aliphatic halogens	Aliphatic halogen	Alkane, branched with quaternary carbon;Alkyl halide;Carboxylic acid ester;Ether moiety;Perfluorocarbon derivatives	Positive(NBHS)																
追加 2-(trifluoromethyl)-2,3,3,3-tetrafluoropropionic acid fluoride	677-84-9		Acyl halides (Genotox)Structural alert for genotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical/Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkane, branched with tertiary carbon;Alkyl halide;Perfluorocarbon derivatives	Positive(NBHS)																
追加 2,3,3,3-tetrafluoro-2-(1,1,2,2-tetrafluoroethyl)thioxypropionic acid fluoride	4089-57-0		Acyl halides (Genotox)Structural alert for genotoxic carcinogenicity	No alert found	AN2,AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical/Radical >> Radical mechanism via ROS formation (indirect);Radical >> Radical mechanism via ROS formation (indirect) >> Geminal Polyhaloalkane Derivatives;SN2,SN2 >> Acylation involving a leaving group after metabolic activation >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> SN2 >> SN2 at sulfur atom;SN2 >> SN2 at sulfur atom >> Sulfonil Halides	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds;Alpha- and beta-Haloether Reactive Functional Groups	Acyl halides	Acyl halides;H-acceptor-path;H-acceptor	Acyl halide;Alkyl halide;Ether moiety;Perfluorocarbon derivatives;Sulfonyl halide	Positive(NBHS)																
追加 2-chloroacryloyl chloride 3,4,4,5,5,6,6-hexafluorohexyl ester	701909-41-3		No alert found	AN2,AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation >> Haloalkene Derivatives with Electron-Withdrawing Groups;AN2 >> Thioacylation via nucleophilic addition after cysteine-mediated thioketene formation >> Polarized Haloalkene Derivatives;SN2,SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation;SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation >> Haloalkene Derivatives with Electron-Withdrawing Groups;SN2 >> Alkylation, direct acting epoxides and related after P450-mediated metabolic activation >> Polarized Haloalkene Derivatives;SN2 >> SN2 at sp3 and activated sp2 carbon atom;SN2 >> SN2 at sp3 and activated sp2 carbon atom >> Nucleophilic addition to alpha,beta-unsaturated carbonyl compounds;AN2 >> Nucleophilic addition to alpha,beta-unsaturated carbonyl compounds >> Propyne Derivatives;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Propyne Derivatives	AN2,AN2 >> Schiff base formation;AN2 >> Schiff base formation >> Polarized Haloalkene Derivatives;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> SN2 >> SN2 at sulfur atom;SN2 >> SN2 at sulfur atom >> Sulfonil Halides	No alert found	Acrylate Reactive Functional Groups;Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Acrylate;Alkene moiety;Alkenyl halide;Alkyl halide;Carboxylic acid ester;Perfluorocarbon derivatives	Positive(NBHS)																
追加 3,3,3-trifluoropropene	661-54-1		No alert found	No alert found	AN2,AN2 >> Nucleophilic addition to alpha,beta-unsaturated carbonyl compounds;AN2 >> Nucleophilic addition to alpha,beta-unsaturated carbonyl compounds >> Propyne Derivatives;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom;SN2 >> Alkylation, nucleophilic substitution at sp3-carbon atom >> Propyne Derivatives	No alert found	Halogenated Linear Aliphatic Hydrocarbon Type Compounds	No alert found	No alert found	Alkyl halide;Alkyne moiety	Positive(NBHS)																

名称	QASRN	構造	Carcinogenicity (genotox and nongenotox) alerts by ISS	DNA alerts for AMES, CA and MNT by OASIS	DNA binding by OASIS	DNA binding by OECD	Oncologic Primary Classification	In vitro mutagenicity (Ames test) alerts by ISS	In vivo mutagenicity (Micronucleus) alerts by ISS	Organic functional groups	遺伝毒性 vitro 複発突然変異試験	遺伝毒性 vitro 染色体異常試験	遺伝毒性 in vitro マウスリンフォーマ試験	In vitro コメット試験	遺伝毒性 vitro 小核試験	遺伝毒性 vitro DNA 鎖切断試験	In vitro HPRTT試験	In vitro 不定期DNA合成試験	In vitro 細胞質転換試験	遺伝毒性 vivo 小核試験	遺伝毒性 vivo DNA損傷	遺伝毒性 in vivo 染色体DNA合成試験	遺伝毒性 in vivo 不定期DNA合成試験	遺伝毒性 in vivo コメット試験	In vivo 突然変異	発がん性
追加 2,2,3,3-tetrafluoroxyetane	765-63-9		No alert found	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Halogenated Oxetanes and Halooxepoxides	SN2;SN2 >> Alkylation, direct acting epoxides and related;SN2 >> Alkylation, direct acting epoxides and related >> Halogenated Oxetanes and Halooxepoxides	No alert found	Alpha- and beta-Haloether Reactive Functional Groups	No alert found	No alert found	Alkyl halide;Ether moiety;Oxetan e;Perfluorocarbon derivatives;Set urated heterocyclic fragment	Positive(NBHS)															
追加 3,4-dichloro-2,2,3,4,4-pentafluorobutyric acid fluoride	678-06-8		Acyl halides (Genotox);Structural alert for genotoxic carcinogenicity	No alert found	AN2;AN2 >> Schiff base formation by aldehyde formed after metabolic activation;AN2 >> Schiff base formation by aldehyde formed after metabolic activation >> Geminal Polyhaloalkane Derivatives;Radical;Radical >> Radical mechanism via ROS Formation (indirect);Radical >> Radical mechanism via ROS Formation (indirect);SN2 >> Acylation involving a leaving group after metabolic activation;SN2 >> Acylation involving a leaving group after metabolic activation >> Geminal Polyhaloalkane Derivatives;SN2 >> DNA alkylation;SN2 >> DNA alkylation >> Vicinal Dihaloalkanes;SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic);SN2 >> Internal SN2 reaction with aziridinium and/or cyclic sulfonium ion formation (enzymatic) >> Vicinal Dihaloalkanes;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation;SN2 >> Nucleophilic substitution at sp3 carbon atom after thiol (glutathione) conjugation >> Geminal Polyhaloalkane Derivatives	Acylation;Acylation >> Direct Addition of an Acyl Halide;Acylation >> Direct Addition of an Acyl Halide >> Acyl halide	Acyl and Benzoyl Type Compounds	Acyl halides	Acyl halides	Acyl halide;Alkyl halide;Perfluorinated carbon derivatives	Positive(NBHS)															
追加 Methanesulfonyl fluoride, trifluoro-	335-05-7		No alert found	SN2;SN2 >> SN2 at sulfur atom;SN2 >> SN2 at sulfur atom >> Sulfonyl Halides	SN2;SN2 >> SN2 at sulfur atom;SN2 >> SN2 at sulfur atom >> Sulfonyl Halides	No alert found	Not classified	No alert found	No alert found	Alkyl halide;Sulfonyl halide	Positive(NBHS)															
Perfluoromethyldodecane	51294-16-7		#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A																
Perfluorodimethylcyclobutane	28677-00-1		#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A																
Perfluoroheptanes (branched and linear)	NOCAS_897718		#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A																