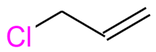
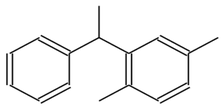
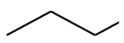
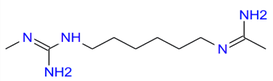
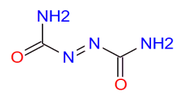
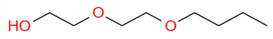
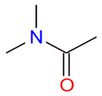
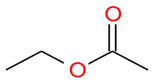
令和８年度生態影響に関する優先度判定　今回新たに有害性クラスの付与を行う物質
人健康影響のみで指定済みの優先評価化学物質　QSAR予測（KATE）

管理番号	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
149	107-05-1 36813-24-8	C=CCCl ３－クロロプロペン （別名塩化アリル） 	1.93	76.52	CNOS_X halogen reactive	Fish	Acute	0.84	in	[-1.77, 4.84]	in	0.36	0.28	1.08	28(7)
					C_X hydrocarbon reactive	Fish	Acute	4.6	out	[2.29, 4.72]	in	0.66	0.43	0.63	9(4)
					C_X hydrocarbon reactive	Daphnid	Acute	11	out	[2.29, 4.63]	in	0.71	0.25	0.56	7(3)
					C_X hydrocarbon reactive excl. 1,3-Dichloropropene	Alga	Acute	310	out	[2.50, 3.44]	in	0.93	-9.74	0.2	3(3)
					C_X hydrocarbon reactive	Daphnid	Chronic	0.51	out	[2.29, 3.44]	in	0.5	-10.07	0.45	4(2)
					C_X hydrocarbon reactive excl. 1,3-Dichloropropene	Alga	Chronic	120	out	[2.50, 3.44]	in	0.97	-4.57	0.18	3(3)
					C_X hydrocarbon reactive	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	1(0)
					CNO_X reactive Fish Chronic	Fish	Chronic	NA	NA	NA	NA	NA	NA	NA	1(0)
220	6165-51-1	CC1=CC(=C(C=C1)C)C(C)C2 =CC=CC=C2 ジメチル（１－ フェニルエチル）ベンゼン 	5.24	210.31	C_X hydrocarbon unreactive aromatic fused R=0 w/o X	Fish	Acute	0.64	in	[1.99, 5.52]	in	0.85	0.79	0.27	24(1)
					narcotic group Fish Acute	Fish	Acute	0.28	in	[-0.63, 5.88]	in	0.87	0.87	0.43	152(33)
					C_X hydrocarbon unreactive aromatic fused R=0 w/o X	Daphnid	Acute	0.44	in	[2.54, 5.52]	in	0.8	0.74	0.23	17(1)
					narcotic group Daphnid Acute	Daphnid	Acute	0.27	in	[1.08, 5.88]	in	0.72	0.71	0.42	81(24)
					narcotic group Alga Acute	Alga	Acute	0.15	in	[1.08, 5.26]	in	0.76	0.73	0.43	51(47)
					C_X hydrocarbon unreactive	Fish	Chronic	0.021	in	[1.52, 5.52]	in	0.78	0.68	0.43	11(0)
					Cnos_X unreactive Fish Chronic	Fish	Chronic	0.018	in	[1.52, 5.52]	in	0.76	0.68	0.43	12(0)
					narcotic group Fish Chronic	Fish	Chronic	0.019	in	[1.52, 5.81]	in	0.82	0.75	0.41	12(0)
					C_X hydrocarbon unreactive aromatic fused R=0 w/o X	Daphnid	Chronic	0.028	in	[2.54, 5.52]	in	0.78	0.71	0.37	15(0)
					narcotic group Daphnid Chronic	Daphnid	Chronic	0.039	in	[-1.20, 5.88]	in	0.78	0.76	0.46	70(12)
					C_X hydrocarbon Alga Chronic	Alga	Chronic	0.15	in	[1.61, 5.52]	in	0.38	0.32	0.61	56(24)
					C_X aromatic hydrocarbon w/o X, biphenyl	Alga	Chronic	0.31	in	[2.54, 5.52]	in	0.55	0.35	0.4	15(1)
					narcotic group Alga Chronic	Alga	Chronic	0.091	in	[0.69, 5.81]	in	0.57	0.53	0.69	58(28)
228	106-94-5	BrCCC １－ブロモプロパン 	2.16	122.99	C_X hydrocarbon unreactive aliphatic w/ X, excl. Halomethane	Fish	Acute	79	in	[1.34, 4.61]	in	0.87	0.86	0.28	24(3)
					CNOS_X halogen unreactive	Fish	Acute	30	in	[0.11, 5.81]	in	0.77	0.75	0.42	96(21)
					narcotic group Fish Acute	Fish	Acute	89	in	[-0.63, 5.88]	in	0.87	0.87	0.43	152(33)
					C_X hydrocarbon unreactive aliphatic w/ X	Daphnid	Acute	18	in	[1.61, 4.52]	in	0.82	0.77	0.3	14(0)
					C_X hydrocarbon unreactive aliphatic w/ X, excl. gem,vic-Cl,TCE	Daphnid	Acute	23	in	[1.98, 4.52]	in	0.98	0.97	0.1	7(0)
					CNOS_X halogen unreactive	Daphnid	Acute	18	in	[0.78, 5.81]	in	0.86	0.85	0.39	46(10)
					narcotic group Daphnid Acute	Daphnid	Acute	20	in	[1.08, 5.88]	in	0.72	0.71	0.42	81(24)
					C_X hydrocarbon unreactive aliphatic w/ X, excl. Halomethane	Alga	Acute	150	in	[1.83, 2.97]	in	0.97	0.91	0.07	5(4)
					CNOS_X halogen unreactive	Alga	Acute	24	in	[0.78, 5.10]	in	0.52	0.47	0.73	34(17)
					narcotic group Alga Acute	Alga	Acute	80	in	[1.08, 5.26]	in	0.76	0.73	0.43	51(47)
					C_X hydrocarbon unreactive	Fish	Chronic	1.7	in	[1.52, 5.52]	in	0.78	0.68	0.43	11(0)
					Cnos_X unreactive Fish Chronic	Fish	Chronic	1.6	in	[1.52, 5.52]	in	0.76	0.68	0.43	12(0)
					narcotic group Fish Chronic	Fish	Chronic	1.8	in	[1.52, 5.81]	in	0.82	0.75	0.41	12(0)
					C_X hydrocarbon unreactive aliphatic w/ X	Daphnid	Chronic	0.8	in	[1.61, 4.52]	in	0.17	-0.09	0.7	13(0)
					C_X hydrocarbon unreactive aliphatic w/ X, excl. gem,vic-Cl,TCE	Daphnid	Chronic	4.4	in	[1.98, 4.52]	in	0.98	0.97	0.09	6(0)
					narcotic group Daphnid Chronic	Daphnid	Chronic	2.1	in	[-1.20, 5.88]	in	0.78	0.76	0.46	70(12)
					C_X hydrocarbon Alga Chronic	Alga	Chronic	5	in	[1.61, 5.52]	in	0.38	0.32	0.61	56(24)
					C_X hydrocarbon unreactive aliphatic w/ X, excl. Halomethane	Alga	Chronic	25	in	[1.83, 2.97]	in	0.48	-0.14	0.43	5(4)
					CNOS_X halogen unreactive	Alga	Chronic	3.7	in	[0.78, 5.81]	in	0.34	0.25	0.9	41(10)
					narcotic group Alga Chronic	Alga	Chronic	9.6	in	[0.69, 5.81]	in	0.57	0.53	0.69	58(28)

管理番号	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
257	32289-58-0	CC(=NCCCCCCNC(=NC)N)N ポリ（アザンジイルカルボノイミドイルアザンジイルカルボノイミドイルアザンジイルヘキサン－１，６－ジイル）のカチオン（窒素原子にプロトンが付加することにより生成したものに限る。）の塩 	1.89	213.32	CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.22	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CN_X imine	Daphnid	Chronic	6.9	in	[-1.34, 3.99]	in	0.95	-1.21	0.15	3(0)
					CN_X imine	Alga	Chronic	1.6	in	[-1.34, 3.99]	in	0.6	-8.93	1.21	4(0)
					CN_X imine	Fish	Acute	180	out(p)	[2.34, 3.99]	in	0.32	-6.42	0.61	4(1)
					CN_X imine	Daphnid	Acute	5	out(p)	[2.89, 3.99]	in	0.03	-272.28	0.14	3(1)
					CN_X imine	Alga	Acute	0.28	out(p)	[2.89, 3.99]	in	0.19	-226.35	0.67	3(1)
264	123-77-3	NC(N=NC(N)=O)=O ジアゼンジカルボキシアミド 	-3.89	116.08	CNO_X azo	Fish	Acute	25000	out	[1.16, 3.63]	in	0.82	-9.7	0.33	3(2)
					urea unreactive	Fish	Acute	8.10E+08	out	[-0.27, 2.67]	in(p)	0.95	0.87	0.24	9(5)
					urea unreactive	Daphnid	Acute	8600	out	[-1.31, 4.90]	in(p)	0.43	-6.71	1.63	3(3)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	14	out	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					urea unreactive	Daphnid	Chronic	1.9	out	[-1.31, 1.95]	in(p)	0.13	-43.49	0.33	3(1)
					urea unreactive	Alga	Chronic	67000	out	[-1.31, 4.90]	out	0.63	-4.09	1.58	3(2)
					CNO_X azo	Alga	Chronic	NA	NA	NA	NA	NA	NA	NA	2(1)
					CNO_X azo	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	1(2)
					urea unreactive	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	2(3)
					CNO_X azo	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(2)
					CNO_X azo	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(1)

管理番号	CAS RN®	SMILES・名称・構造式	log P (Estimated)	MW	QSAR Class	Type of Predicted Toxicity		Predicted Toxicity [mg/L]	Applicability Domain Judgement			Statistics of QSAR Regression			
						Organism	Acute or Chronic		Log P [Range]		structure	R^2	Q^2	RMSE	n
276	112-34-5	CCCCOCCOCCO ２－（２－ブトキシエトキシ）エタン－１－オール （別名ジエチレングリコールモノブチルエーテル） 	0.29	162.23	CO_X primary alcohol	Fish	Acute	5500	in	[-1.75, 5.26]	in	0.92	0.9	0.44	22(15)
					CO_X ether unreactive	Fish	Acute	4000	in	[-1.75, 5.10]	in	0.87	0.86	0.52	44(17)
					CO_X alcohol unreactive w/ EO	Fish	Acute	2800	in	[-1.75, 3.22]	in	0.98	0.97	0.19	5(6)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.63	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CO_X ether unreactive	Daphnid	Chronic	92	in	[0.00, 4.66]	in	0.88	0.76	0.58	10(8)
					alcohol unreactive w/ EO alga	Alga	Chronic	76	in	[0.02, 3.22]	in	0.88	-1.81	0.34	4(3)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Chronic	110	in	[0.02, 5.13]	in	0.74	0.69	0.56	19(10)
					CO_X primary alcohol	Daphnid	Acute	2100	out(p)	[2.31, 5.26]	in	0.95	0.76	0.17	6(17)
					CO_X ether unreactive	Daphnid	Acute	4100	out(p)	[1.34, 5.13]	in	0.75	0.69	0.59	19(19)
					CO_X primary alcohol	Alga	Acute	28000	out(p)	[2.31, 5.26]	in	0.91	0.79	0.36	6(16)
					CO_X ether unreactive excl. HRAC Ea Alga	Alga	Acute	7300	out(p)	[1.34, 5.10]	in	0.68	0.58	0.6	12(17)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Acute	NA	NA	NA	NA	NA	NA	NA	0(7)
					alcohol unreactive w/ EO alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(6)
					CO_X alcohol unreactive w/ EO Daphnid	Daphnid	Chronic	NA	NA	NA	NA	NA	NA	NA	2(4)
277	127-19-5	CC(N(C)C)=O Ｎ，Ｎ－ジメチルアセトアミド 	-0.49	87.12	CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.64	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					CNO_X amide unreactive Daphnid	Daphnid	Chronic	65	in	[-1.61, 5.62]	in	0.83	0.74	0.55	8(6)
					CNO_X amide unreactive Alga	Alga	Chronic	33	in	[-1.61, 5.62]	in	0.56	-0.18	0.3	6(7)
					CNO_X amide unreactive	Fish	Acute	670	out(p)	[0.27, 5.62]	in	0.8	0.76	0.37	21(8)
					CNO_X amide unreactive Daphnid	Daphnid	Acute	16000	out(p)	[0.99, 5.62]	in	0.88	0.7	0.51	6(9)
					CNO_X amide unreactive Alga	Alga	Acute	NA	NA	NA	NA	NA	NA	NA	1(12)
278	141-78-6	CC(OCC)=O 酢酸エチル 	0.86	88.11	CNO_X ester unreactive	Fish	Acute	65	in	[0.37, 4.61]	in	0.72	0.68	0.43	37(21)
					CNO_X ester unreactive Daphnid	Daphnid	Acute	130	in	[0.36, 5.28]	in	0.93	0.86	0.3	8(17)
					CNO_X unreactive Fish Chronic, w/ N,O	Fish	Chronic	0.21	in	[-1.61, 5.99]	in	0.62	0.54	0.57	19(2)
					ester unreactive w/o acid	Daphnid	Chronic	12	in	[0.59, 5.28]	in	0.81	0.69	0.42	9(19)
					CNO_X ester unreactive Daphnid	Daphnid	Chronic	15	in	[0.59, 5.28]	in	0.84	0.73	0.4	8(18)
					ester unreactive w/o acid	Alga	Chronic	160	in	[0.36, 5.28]	in	0.88	0.79	0.51	9(19)
					CNO_X ester unreactive Alga	Alga	Chronic	190	in	[0.36, 5.28]	in	0.9	0.79	0.49	8(17)
					CNO_X ester unreactive Alga	Alga	Acute	790	out(p)	[1.77, 5.28]	in	0.94	0.85	0.33	6(19)