

## 既存化学物質の生態影響に関する情報

(平成18年12月22日開催)

官報公示 整理番号	CAS No.	物質名称	頁
2-240	126-30-7	2, 2-ジメチル-1, 3-プロパンジオール	1
3-790	2581-34-2	3-メチル-4-ニトロフェノール	13
3-969	58-90-2	2, 3, 4, 6-テトラクロロフェノール	30
4-645	83-32-9	アセナフテン	43
3-41	541-73-1	m-ジクロロベンゼン	56
4-852 4-854	6362-80-7	2, 4-ジフェニル-4-メチルペンテン-1	66
3-965 3-987	30171-80-3	ジブロモクレジルグリシジルエーテル	77

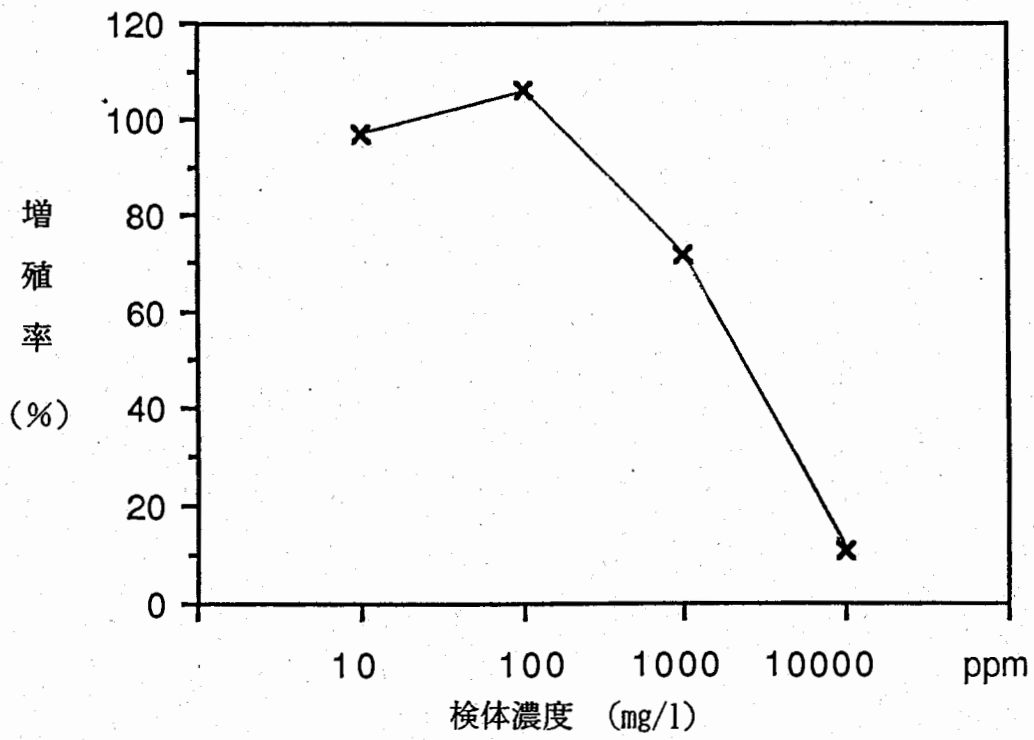


図1-4 セレナストルムの増殖に対する  
2,2-ジメチル-1,3-プロパンジオールの効果 (予試)

表2-7 予備試験

<2,2-ジメチル-1,3-7°ロハ°ンジオール>

	化合物 濃度 (mg/l)	分散剤 濃度 (mg/l)	p H		D O		遊泳阻害数					阻害率 (%)
			試験前	試験後	試験前	試験後	1	2	3	4	計	
1	1	-	6.66	6.65	9.70	8.90	0	1	0	1	2	10
2	10	-	6.68	5.57	9.37	8.43	0	0	0	0	0	0
3	100	-	6.65	6.96	9.61	8.58	0	1	1	0	2	10
4	1000	-	6.80	6.87	9.23	7.18	0	0	0	0	0	0
B L	-	-	6.65	6.67	9.47	8.81	0	0	0	1	1	5

2-2-ジメチル-1,3-プロパンジオール

阻害率  
%

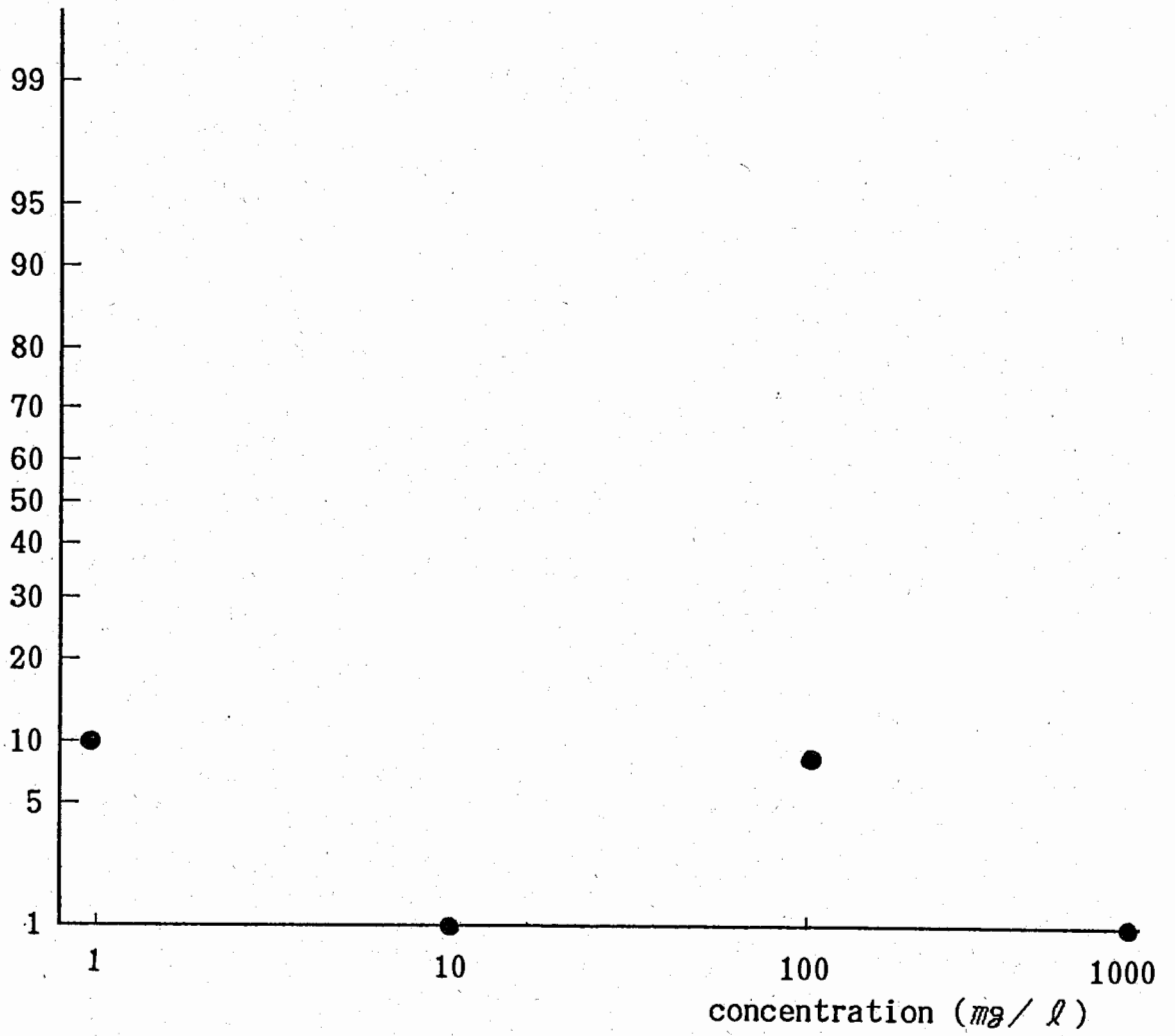


図2-5 各濃度の遊泳阻害率 (EC<sub>50</sub>)

表2-15 繁殖試験結果

2,2-ジメチル-1,3-プロピオンジオール

濃度 (mg/l)		日																					
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	
1	1000	生存数	39	37	37	34	34	34	35	34	34	34	34	34	34	34	34	34	34	34	34	34	33
		産仔数	0	0	0	0	0	0	10	61	90	133	130	202	141	246	247	117	106	147	5		
2	320	生存数	39	39	39	38	38	37	37	36	36	36	36	36	36	36	35	35	35	35	35	35	35
		産仔数	0	0	0	0	0	0	52	140	94	152	232	144	89	250	229	0	142	181	53		
3	100	生存数	40	40	40	39	39	39	37	35	37	36	35	34	35	35	35	35	35	35	35	35	35
		産仔数	0	0	0	0	0	0	48	70	131	171	112	184	183	159	209	46	108	181	22		
4	32	生存数	40	38	38	38	35	35	34	33	34	34	34	34	34	34	33	33	33	33	33	33	33
		産仔数	0	0	0	0	0	0	57	161	78	179	195	163	257	202	182	122	94	121	30		
5	10	生存数	40	40	39	39	39	39	39	39	38	38	38	38	38	36	37	37	37	37	37	36	36
		産仔数	0	0	0	0	0	0	198	62	64	316	34	123	170	278	107	19	183	59	54		
BL	BL	生存数	39	38	36	36	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35	35
		産仔数	0	0	0	0	0	0	133	130	114	177	184	165	199	197	168	26	119	141	49		

④ 2, 2-ジメチル-1, 3-プロパンジオール

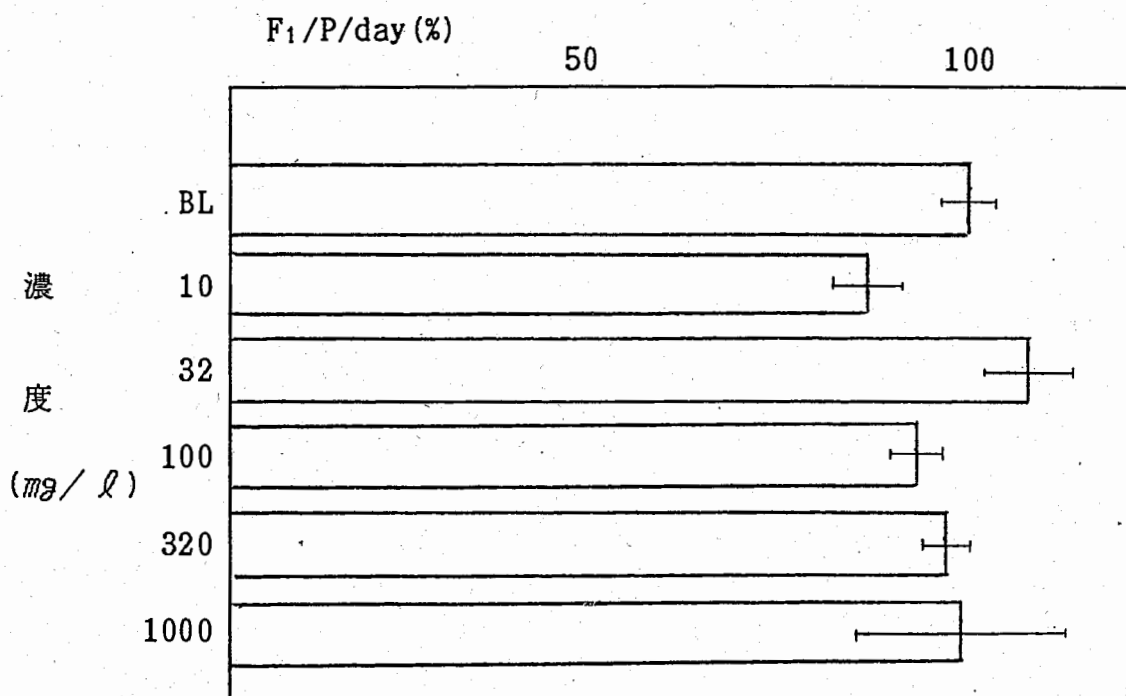


図2-11 濃度別産仔数 (F<sub>1</sub>/P/day) の平均値及び有意差  
 (\*:5%の危険率で有意差あり)

表3-6 ヒメダカ急性毒性試験

供試化学物質 2,2-ジメチル-1,3-プロパンジオール

試験温度 22°C 脱塩素水系を使用, 溶解補助剤:

No.	化合物 mg/L	補助剤 mg/L	24 時間			48 時間			72 時間			96 時間		
			生存数	pH	DO	生存数	pH	DO	生存数	pH	DO	生存数	pH	DO
1	1,000	0	9	7.6 7.2	8.7 2.8	9	7.6 7.2	8.9 4.1	9	7.7 7.3	9.0 4.6	9	7.6 7.4	8.8 4.6
2	555	0	10	7.7 7.3	8.8 3.3	10	7.7 7.3	8.9 5.0	10	7.8 7.4	9.0 4.9	10	7.7 7.4	8.9 4.9
3	309	0	10	7.7 7.3	8.9 3.3	10	7.8 7.4	9.0 4.6	10	7.9 7.4	9.1 4.3	10	7.8 7.4	9.0 4.8
4	171	0	10	7.7 7.3	8.9 3.8	10	7.8 7.5	9.0 5.0	10	7.9 7.4	9.2 5.0	10	7.9 7.5	9.0 5.2
5	95	0	10	7.7 7.4	8.9 4.3	10	7.8 7.5	8.8 5.4	10	7.8 7.5	9.1 5.4	10	7.9 7.5	9.0 5.6
B1														
B2	0	0	10	7.7 6.8	8.8 4.3	10	7.8 7.5	8.9 5.2	10	8.0 7.6	8.9 5.6	10	8.0 7.0	8.9 5.1
LC <sub>50</sub> (mg/L)			>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000	>1,000
死亡率 100%最低濃度			—	—	—	—	—	—	—	—	—	—	—	—
死亡率 0%最高濃度			555	555	555	555	555	555	555	555	555	555	555	555
コメント (魚の状態, 沈 澱の有無など)														

pH, DOは上段が飼育前, 下段が飼育後。

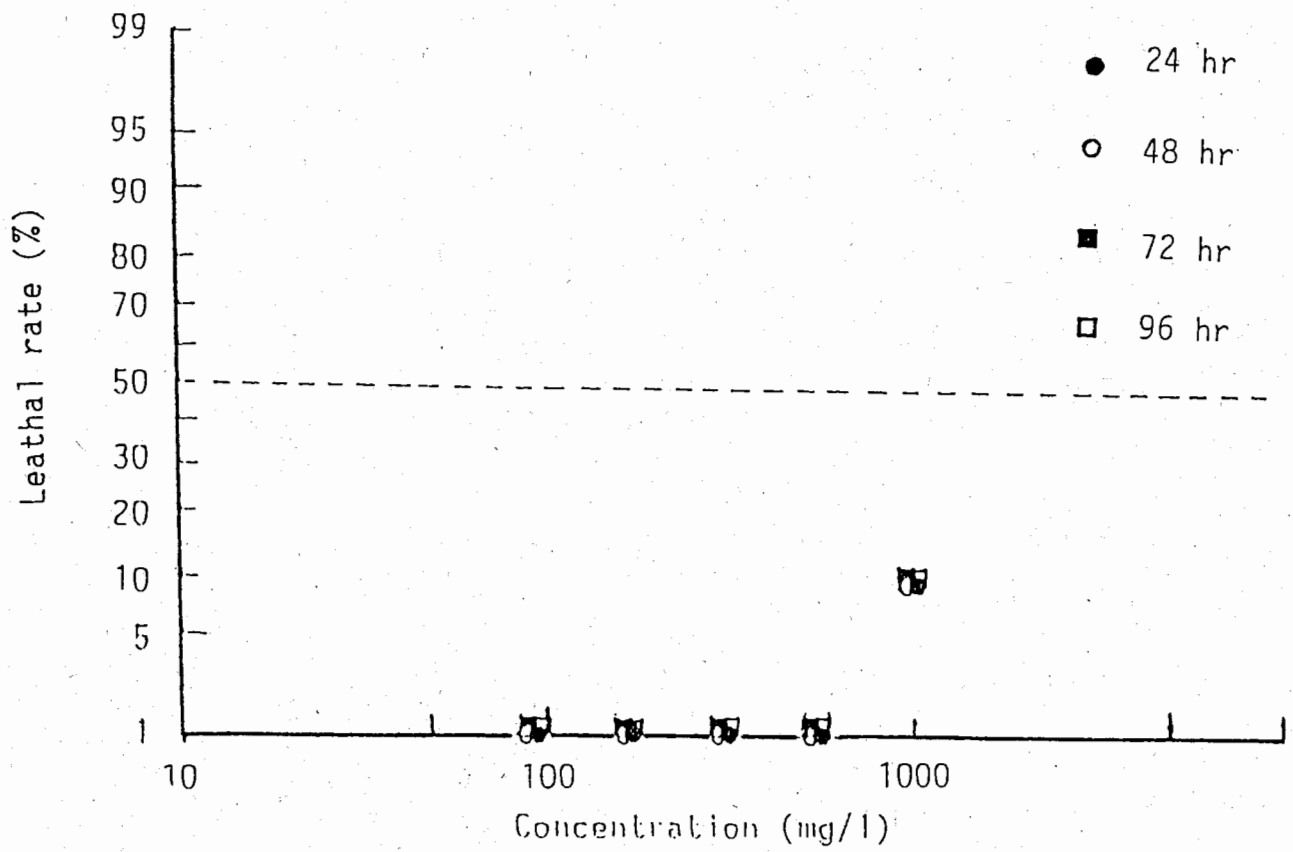


図3-4 ヒメダカ急性毒性試験における  
2,2-ジメチル-1,3-プロパンジオールの濃度と死亡率との関係



## Study

End Point : **AQUATIC ACUTE TOXICITY**  
 Chemical Name : **1,3-Propanediol, 2,2-dimethyl**  
 CAS Number : **126-30-7**

Species/strain/system : Orange-red Killifish (*Oryzias latipes*)  
 Exposure Period : **24-96 h**  
 Exposure comments : The same doses were also tested for 48h and 72h.

## Test Method and Conditions

Test method description : Semi-static

## Test Results

<u>Organism</u>	<u>Medium</u>	<u>Spec.</u>	<u>Route</u>	<u>Lifestage</u>	<u>Sex</u>	<u>Effect</u>	<u>Effect Comments</u>
<b>FISH</b>	<b>AQ</b>	<b>ESTUA</b>				<b>LC0</b>	LC0 = 555mg/l (reported as 555ppm)
						<b>LC50</b>	for 24, 48, 72 and 96 hours, LC50 = > 1000mg/l (reported as > 1000ppm (w/v)).

## References

Primary Reference : **#UREAF\***  
 Unpublished Report on Toxicity to Fish Test conducted by Environmental Agency, Japan

Secondary Reference : **ISIDSP\***  
 OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

## Study

End Point : **AQUATIC ACUTE TOXICITY**  
 Chemical Name : **1,3-Propanediol, 2,2-dimethyl**  
 CAS Number : **126-30-7**

Species/strain/system : Orange-red Killifish (*Oryzias latipes*)  
 Exposure Period : **48 h**

## Test Substance

Impurities : **Water 0.03%, neopentyl hydroxy pivalate 0.44%, formic acid 0.002%**

## Test Method and Conditions

Test method description : JIS K0102. Static test.

## Test Results

<u>Organism</u>	<u>Medium</u>	<u>Spec.</u>	<u>Route</u>	<u>Lifestage</u>	<u>Sex</u>	<u>Effect</u>	<u>Effect Comments</u>
<b>FISH</b>	<b>ESTUA</b>					<b>LC50</b>	> 1000mg/l (reported > 1000 ppm)

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## References

- Primary Reference* : **#UREAF\***  
Unpublished Report on Toxicity to Fish Test conducted by Environmental Agency, Japan
- Secondary Reference* : **!SIDSP\***  
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)
-

## Study

End Point : **AQUATIC TOXICITY**  
 Chemical Name : **1,3-Propanediol, 2,2-dimethyl-**  
 CAS Number : **126-30-7**

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

**ALGAE**

Species/strain/system : Algae (Selenastrum capricornutum)

## Test Substance

Description of the test substance : Neopentyl glycol  
 Purity Grade : **>99%**

## Test Method and Conditions

Test method description : OECD Test Guideline. GLP: no

## Exposure

Exposure Period : **72 h**  
 Dose / Concentration : **>1000 mg/l, w/v**

## Test Results

<u>Organ</u>	<u>Effect</u>	<u>Rev.</u>	<u>OnSet</u>	<u>Sex</u>	<u>Affected in Exposed - Controls</u>
	<b>EC50</b>				
Effective concentration (reported as EBC50 > 1000ppm (w/v) for 42h)					

## References

Primary Reference : **#UREAA\***  
 Unpublished Report on Toxicity to Algae Test conducted by Environmental Agency, Japan, (1993)

Secondary Reference : **!SIDSP\***  
 Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

## Study

End Point : **AQUATIC TOXICITY**  
 Chemical Name : **1,3-Propanediol, 2,2-dimethyl**  
 CAS Number : **126-30-7**

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

**CRUS**  
**AQ**

Species/strain/system : Water flea (Daphnia magna)

## Test Substance

Purity Grade : **98%**

## Test Method and Conditions

Test method description : Static test. Method used to calculate EC values: Probit method.

## Exposure

Exposure Period : **21 d**  
**24-48 h**

## Test Results

<u>Organ</u>	<u>Effect</u>	<u>Rev.</u>	<u>OnSet</u>	<u>Sex</u>	<u>Affected in Exposed - Controls</u>
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### **NOEC**

Maximum concentration at which no effect was observed > 1000ppm (w/v) for 21 days.

### **EC0**

For 24h lowest dose without effect: > 1000ppm (w/v)

### **EC50**

For 24h lowest dose without effect: > 1000ppm (w/v)

## References

Primary Reference : **#URTEA\***  
 Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan

Secondary Reference : **!SIDSP\***  
 OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

## Study

End Point : **AQUATIC TOXICITY**  
 Chemical Name : **1,3-Propanediol, 2,2-dimethyl-**  
 CAS Number : **126-30-7**

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

**CRUS**

Species/strain/system : Water flea (Daphnia magna)

## Test Substance

Description of the test substance : Neopentyl glycol  
 Purity Grade : >98%

## Test Method and Conditions

Test method description : GLP: no. Probit method used to calculate these values.

## Exposure

Exposure Type : **ACUTE**  
 Exposure Period : **24-48 h**  
 Dose / Concentration : **>1000 ppm w/v**

## Test Results

<u>Organ</u>	<u>Effect</u>	<u>Rev.</u>	<u>OnSet</u>	<u>Sex</u>	<u>Affected in Exposed - Controls</u>
	<b>EC0</b>				

**EC50**

The 24h EC0 and EC50 are higher than 1000ppm w/v.

## References

Primary Reference : **#URTEA\***  
 Unpublished Toxicity Test conducted by the Environmental Agency, (EA), Japan, (1993)

Secondary Reference : **ISIDSP\***  
 Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1993)

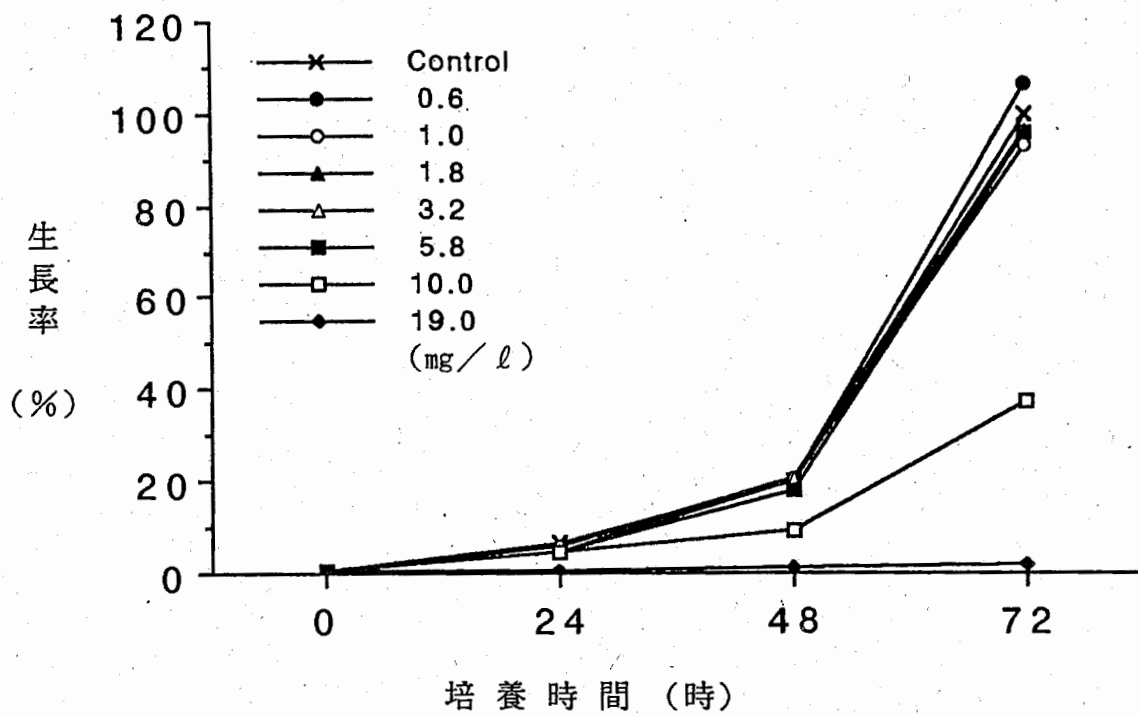


図1-20. 3-メチル-4-ニトロフェノールの各濃度におけるセレナストルムの生長曲線 (岐阜県公害研究所)

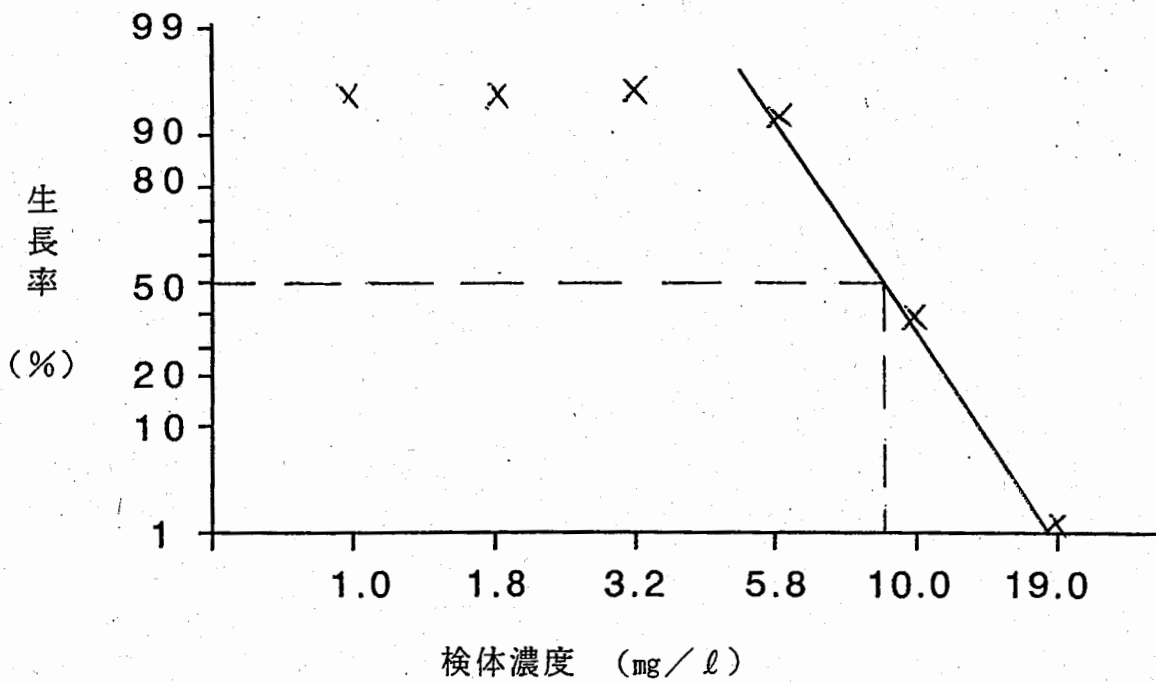


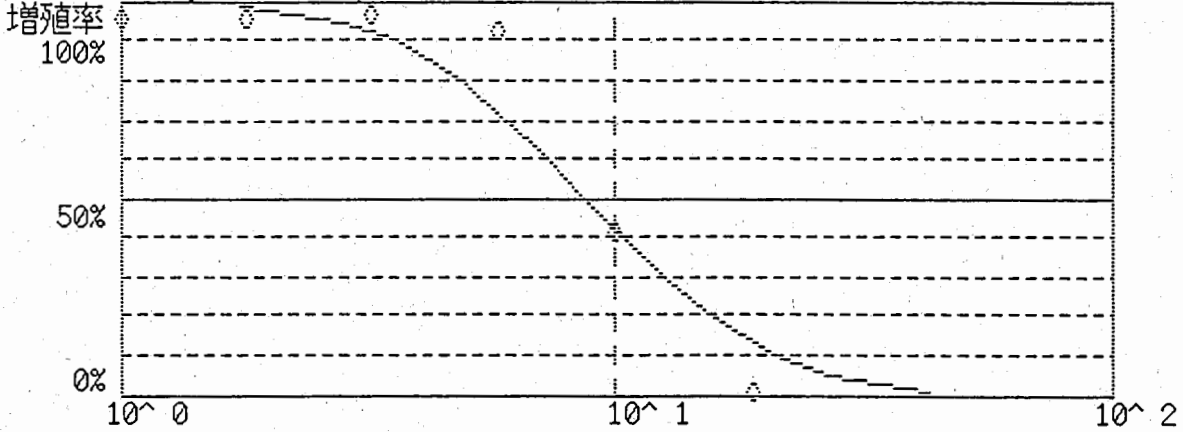
図1-36. セレナストルムの生長に対する3-メチル-4-ニトロフェノールの効果 (本試) (岐阜県公害研究所)

No. = 40 ; 3-Methyl-4-Nitrophenol

Probit(Y) = 8.1304 + -3.3414 LOG10(X) N = 6  
 95%信頼限界 9.327 <=LC50( 8.647) <= 8.044 t0.05 = 1.96  
 LC95 = 2.783 LC90 = 3.575 LC80 = 4.841 LC70 = 6.024 LC60 = 7.262 LC50 = 8.647  
 LC40 = 10.29 LC30 = 12.41 LC20 = 15.44 LC10 = 20.91 LC 5 = 26.86

No.	濃度 (X)	標準値	増殖値 (%)	濃度 log(X)	増殖率 Probit	予測 Probit
1	1	178	171 (96.1%)	0.000	6.759	8.130
2	1.8	178	171 (96.1%)	0.255	6.759	7.277
3	3.2	178	172 (96.6%)	0.505	6.830	6.443
4	5.8	178	165 (92.7%)	0.763	6.455	5.580
5	10	178	73 (41.0%)	1.000	4.774	4.789
6	19	178	2 (1.1%)	1.279	2.719	3.858

No. 40 3-Methyl-4-Nitrophenol



濃度	1	1.8	3.2	5.8	10	19
標準値	178	178	178	178	178	178
増殖値	171	171	172	165	73	2
増殖率(%)	96	96	96.6	92.6	41	1.1

Probit(Y) = 8.1304 + -3.3414 log10(X) n = 6  
 95%信頼限界 9.327 <=LC50( 8.647) <= 8.044 t0.05 = 1.96  
 LC95 = 2.783 LC90 = 3.575 LC80 = 4.841 LC60 = 7.262 LC50 = 8.647  
 LC40 = 10.29 LC20 = 15.44 LC10 = 20.91 LC 5 = 26.86

図1-49. セレナストルムの生長に対する  
 3-メチル-4-ニトロフェノールの効果  
 (本試. プロビット法)

表 2-12

予備試験 <3-メチル-4-ニトロフェノール>

試験機関名：福岡県保健環境研究所

	化学物質濃度 mg/l	分散剤濃度 mg/l	pH		DO		遊泳阻害(数)					阻害率 (%)
			試験前	試験後	試験前	試験後	1	2	3	4	計	
1	0.1	—	7.5	7.7	9.1	8.8	0	0	0	0	0	0
2	1	—	7.6	7.7	9.0	8.8	1	0	0	0	1	5
3	10	—	7.4	7.7	9.0	8.8	1	3	2	2	8	40
4	100	—	6.9	6.9	9.0	9.0	5	5	5	5	20	100
5	1000	—	6.2	6.2	7.6	7.6	5	5	5	5	20	100
BL	—	—	7.5	7.6	9.1	8.8	0	0	0	0	0	0

本試験 <3-メチル-4-ニトロフェノール>

試験機関名：福岡県保健環境研究所

	化学物質濃度 mg/l	分散剤濃度 mg/l	pH		DO		遊泳阻害(数)					阻害率 (%)
			試験前	試験後	試験前	試験後	1	2	3	4	計	
1	3.2	—	7.6	7.5	8.9	8.7	0	0	0	0	0	0
2	5.6	—	7.6	7.6	9.0	8.7	0	0	1	0	1	5
3	10	—	7.6	7.7	9.0	8.6	3	4	3	2	12	60
4	18	—	7.4	7.7	9.0	8.7	5	5	5	5	20	100
5	32	—	7.3	7.7	9.0	8.8	5	5	5	5	20	100
BL	—	—	7.6	7.2	9.1	8.8	0	0	0	0	0	0



3-メチル-4-ニトロフェノール

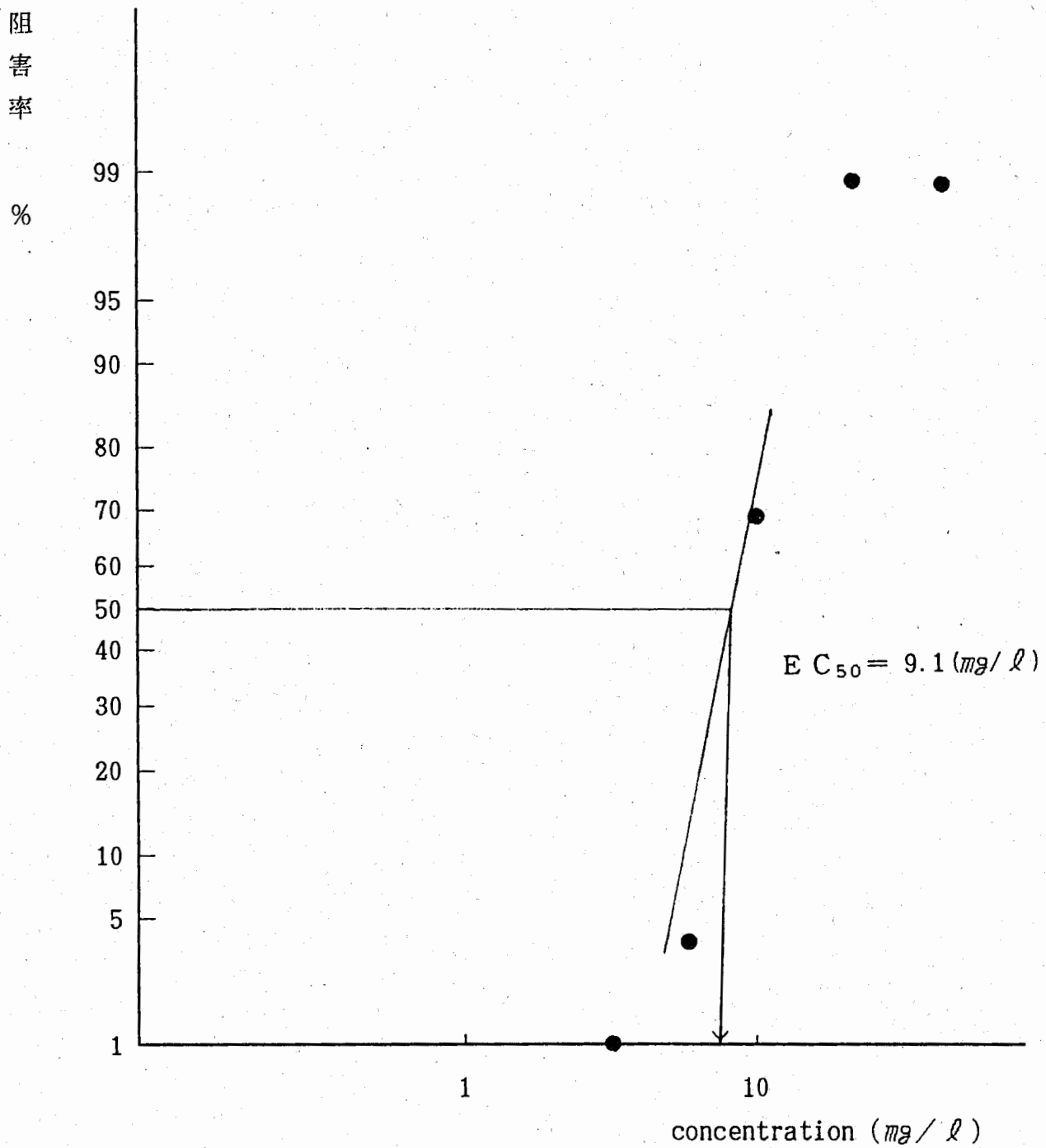


図2-10 各濃度の遊泳阻害率 ( $EC_{50}$ )  
(福岡県保健環境研究所)



表 2-36 累積産仔率及び対照区との有意差の有無  
 〈3-メチル-4-ニトロフェノール〉

No.	対 照	濃 度 (mg/ℓ)				
		1	1.8	* 3.2	* 5.6	* 10
1	69.4(8)	63.5(8)	79.8(10)	46.6(9)	11.7(16)	0 (-)
2	71.9(9)	93.3(9)	85.0(9)	41.6(9)	16.7(14)	0 (-)
3	62.5(8)	78.3(9)	92.8(9)	52.2(9)	17.6(14)	0 (-)
4	73.0(10)	84.6(9)	67.9(8)	46.4(9)	4.15(14)	0 (-)
平 均	69.2	79.9	81.4	46.5	12.5	0
標準偏差	4.70	12.6	10.4	4.38	6.17	0

\* : 5%危険立において有意差有り  
 ( ) 内は初産日を示した。

⑦ 3-メチル-4-ニトロフェノール

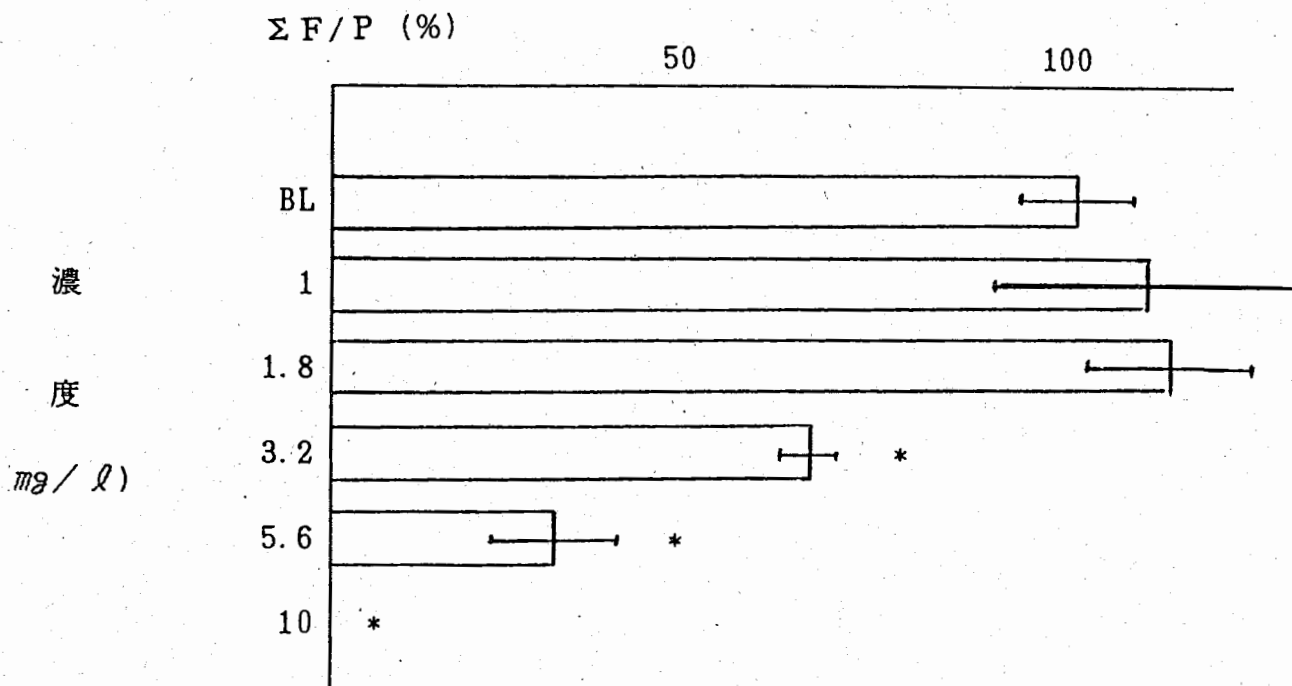


図 2-19 濃度別累積産仔数 (Σ F/P) の平均値及び有意差  
 (\* : 5%の危険率で有意差あり)

表3-11 ヒメダカ急性毒性試験結果

供試化学物質：3-メチル-4-ニトロフェノール

試験機関名：福岡県保健環境研究所

No.	試験溶液量 (ml)	供試化学物質濃度 (mg/l)	溶解補助剤濃度 (ml/l)	供試魚数	24時間			48時間			72時間			96時間			死亡率100%最低濃度 (mg/l)
					生存数	pH	DO	生存数	pH	DO	生存数	pH	DO	生存数	pH	DO	
1	3,000	18	—	10	0	7.3	8.6	0	—	—	—	0	—	—	—	—	18
						7.2	7.9										
2	3,000	10	—	10	9	7.5	8.6	3	7.5	8.7	3	7.2	8.6	3	7.5	8.7	他の観察された影響とそれらが認められた濃度 (mg/l)
						7.0	4.6			6.8		4.9			7.1	6.0	
3	3,000	5.6	—	10	10	7.5	8.7	10	7.5	8.7	10	7.2	8.6	10	7.5	8.7	
						7.1	5.1			6.7		4.1			7.0	4.9	
4	3,000	3.1	—	10	10	7.5	8.5	10	7.6	8.7	10	7.3	8.6	10	7.6	8.6	
						7.0	5.2			6.8		4.5			7.0	5.4	
5	3,000	1.8	—	10	10	7.6	8.6	10	7.6	8.7	10	7.3	8.5	10	7.6	8.6	
						7.0	5.6			6.8		5.2			7.0	5.5	
B1	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—
B2	3,000	—	—	10	10	7.4	8.6	10	7.5	8.8	10	7.1	8.7	10	7.6	8.6	—
						7.0	5.4		6.8	5.6		7.0	5.0		6.9	6.1	
L C <sub>50</sub> 値 (mg/l)					11	9.8			9.8			9.8					
L C <sub>50</sub> 値の95%信頼限界					3.3 ≤ X ≤ 36	5.8 ≤ X ≤ 16			5.8 ≤ X ≤ 16			5.8 ≤ X ≤ 16					

備考：

pH, DOは上段が飼育前, 下段が飼育後

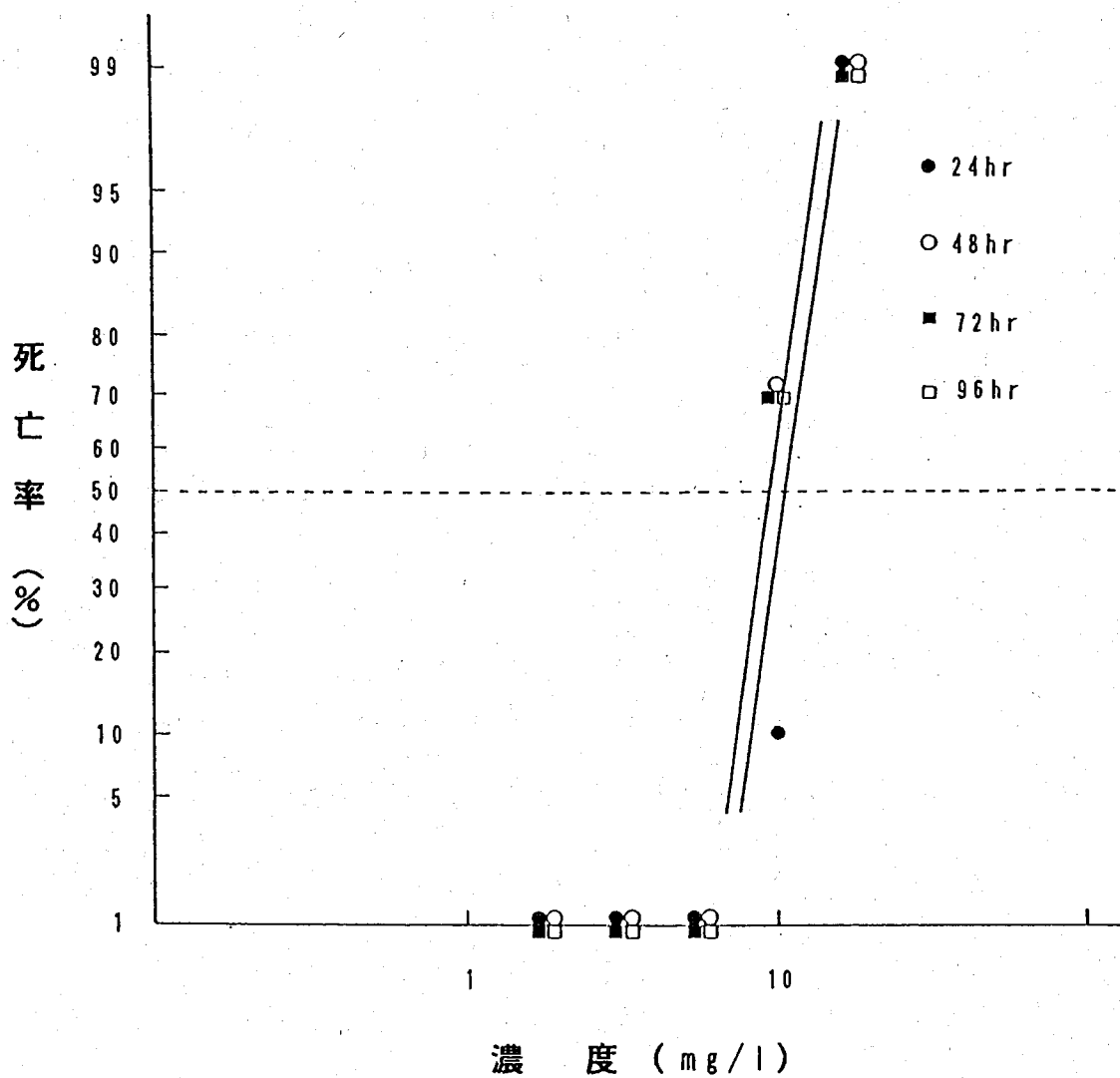
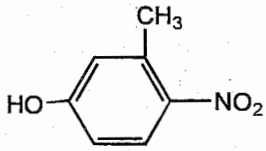


図 3-10 ヒメダカ急性毒性試験における  
3-メチル-4-ニトロフェノールの濃度と死亡率との関係  
(福岡県保健環境研究所)

**SIDS INITIAL ASSESSMENT PROFILE**

CAS No.	2581-34-2
Chemical Name	Phenol, 3-methyl-4-nitro-
Structural Formula	

**CONCLUSIONS AND RECOMMENDATIONS**

Potential risk to man is identified due to genotoxicity and thus presumed carcinogenicity, but measures currently in place reduce risks such that the chemical is of low priority for further work.

**SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS**

3-Methyl-4-nitrophenol is a stable solid, and the production volume was 3,300 tonnes/year for 1990 - 1993 in Japan. The substance is used as an intermediate for the synthesis of pesticides. Based on an international information gathering activity on exposure, 3-methyl-4-nitrophenol has been produced in two OECD Member countries, i.e. Japan and Denmark. In Japan, the chemical is manufactured and processed in a closed system, i.e. the product itself and all reagents and solvents for its synthesis are handled in perfectly closed tubes and vessels. The synthesis is operated within the same plant. At the work place, protective clothing, gloves and goggles are used. No consumer uses are known. Monitoring data in the general environment in Japan (surface water and sediments) are available, but the substance was not detected in 1984. Regarding the Japanese global situation, the predicted worst case concentration in surface water is  $1.7 \times 10^{-4}$  mg/l and the predicted indirect exposure to humans through the environment was calculated to be  $1.4 \times 10^{-3}$  mg/man/day (i.e.  $2.3 \times 10^{-5}$  mg/kg/day). In Denmark, the chemical is produced, but detailed exposure information is not available, except that there is no consumer use.

For the environment, various NOEC and LC<sub>50</sub> values were gained from test results; LC<sub>50</sub> = 9.8 mg/l (acute fish); EC<sub>50</sub> = 9.1 mg/l (acute daphnia); EC<sub>50</sub> = 8.6 mg/l (acute algae); NOEC = 0.78 mg/l (long-term daphnia reproduction). Therefore, the chemical is considered to be moderately toxic to fish, daphnids and algae. The lowest chronic toxicity result, 21 d-NOEC (reproduction) of *Daphnia magna* (0.78 mg/l), was adopted for the calculation of the PNEC, applying an assessment factor of 100. Thus the PNEC of the chemical is 0.0078 mg/l. Since the PEC is lower than the PNEC, the environmental risk is presumably low.

The chemical showed genotoxic effects in a chromosomal aberration test *in vitro* and in an *in vivo* micronucleus test. In a 6 months repeated dose toxicity test, the chemical showed a transient excretion of glucose to urine in the 1500 ppm group, but no other abnormalities were noted. In an OECD preliminary reproductive/developmental toxicity test, the chemical showed no effect on reproductive ability, organ weight, histopathological appearance of reproductive organs, delivery and maternal behaviour of dams, viability, clinical signs, body weight change and autopsy findings for offspring. Also, as repeated dose effect to male rats, decreased locomotor activity, prone position, bradypnea and thrombus in the kidney, heart and lung were observed in the high-dose group (300 mg/kg/day). The NOEL for 6 months repeated dose toxicity was 500 ppm (30.7 mg/kg/day) in both sexes. The NOEL for reproductive toxicity was 300 mg/kg/day and the NOEL for repeat dose toxicity to male rats in the preliminary reproductive test was 100 mg/kg/day.

3-Methyl-4-nitrophenol showed genotoxicity in an *in vitro* chromosomal aberration test. However, this chemical is used as raw material for the synthesis of pesticides in closed systems, and the results from gathering international exposure information showed that the production volume is low, and exposure to the general population from the general environment is currently low. In Japan, the chemical is manufactured and processed in a closed system, i.e. the product itself and all reagents and solvents for its synthesis are handled in perfectly closed tubes and vessels. The synthesis is operated within the same plant. At the work place, protective clothing, gloves and goggles are used. The

daily intake of the chemical via the environment was estimated to be  $1.4 \times 10^{-3}$  mg/man/day (i.e.  $2.3 \times 10^{-5}$  mg/kg/day) from the result of worst-case calculation using the MNSEM 145I exposure model. The concentrations in surface water and sediments were not detectable in a Japanese environmental monitoring program. No consumer uses have been identified. Although no data on work place monitoring have been reported, voluntary exposure reducing procedures are in place in Japan. Occupational exposure seems to be low.

Therefore, 3-methyl-4-nitrophenol is considered as low priority for further work.

#### NATURE OF FURTHER WORK RECOMMENDED

## FULL SIDS SUMMARY

## 3-Methyl-4-nitrophenol

CAS NO: 2581-34-2		SPECIES	PROTOCOL	RESULTS
<b>PHYSICAL-CHEMICAL</b>				
2.1	Melting Point			133 – 133.5 °C
2.2	Boiling Point			207 °C
2.3	Density			No data available
2.4	Vapour Pressure		OECD TG 104	< 5.2 x 10 <sup>-4</sup> hPa at 100 °C
2.5	Partition Coefficient (Log Pow)		OECD TG 107	2.12 at 25 °C
2.6 A.	Water Solubility		OECD TG 105	13 mg/L at 25 °C
B.	pH			No data available.
	pKa			Not observed.
2.12	Oxidation: Reduction Potential			No data available.
<b>ENVIRONMENTAL FATE AND PATHWAY</b>				
3.1.1	Photodegradation		Estimation	T <sub>1/2</sub> = 1.35 y (direct photolysis in water)
3.1.2	Stability in Water		OECD TG 111	Stable at pH 4.0, 7.0, 9.0
3.2	Monitoring Data			In Japanese monitoring study, not detected from surface water and sediment in 1984.
3.3	Transport and Distribution		Calculated (MNSEM-147S)	In Air 1.8E-9 mg/L In Water 1.7E-4 mg/L In Soil 4.1E-3 mg/g In Sediment 6.8E-3 mg/g
3.5	Biodegradation		OECD TG 301C	Not readily biodegradable: 0% (BOD) in 28 days, 3 % (TOC), 6 % (UV) in 28 days
3.6	Bioaccumulation	Carp	OECD TG 305C	BCF: 5.2 – 31
<b>ECOTOXICOLOGY</b>				
4.1	Acute/Prolonged Toxicity to Fish	<i>Oryzias latipes</i>	OECD TG 203	LC <sub>50</sub> (24hr): 11 mg/L LC <sub>50</sub> (96hr): 9.8 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates ( <i>Daphnia</i> )	<i>Daphnia magna</i>	OECD TG 202	EC <sub>50</sub> (24hr): 9.1 mg/l
4.3	Toxicity to Aquatic Plants e.g. Algae	<i>Selenastrum capricornutum</i>	OECD TG 201	EC <sub>50</sub> (72hr): 8.6 mg/l NOEC: 5.8 mg/l
4.5.2	Chronic Toxicity to Aquatic Invertebrates ( <i>Daphnia</i> )	<i>Daphnia magna</i>	OECD TG 202	LC <sub>50</sub> (21d, Mortality): 2.9 mg/l LC <sub>50</sub> (21d, Reproduction): 3.9 mg/l NOEC (21d, Repro): 0.78 mg/l
4.6.1	Toxicity to Soil Dwelling Organisms			No data available.
4.6.2	Toxicity to Terrestrial Plants			No data available.
(4.6.3)	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)			No data available
<b>TOXICOLOGY</b>				
5.1.1	Acute Oral Toxicity	Rat	Unknown	LD <sub>50</sub> : 1,200 mg/kg (female) LD <sub>50</sub> : 2,300 mg/kg (male)
5.1.2	Acute Inhalation Toxicity			No data available.
5.1.3	Acute Dermal Toxicity			No data available.
5.4	Repeated Dose Toxicity	Rat	Oral (diet) 6 month	NOEL = 30.7 mg/kg/day



CAS NO: 2581-34-2		SPECIES	PROTOCOL	RESULTS
5.5	Genetic Toxicity In Vitro	<i>S. typhimurium</i> <i>E. coli</i>	OECD Guidelines No.471 and 472 and Japanese Guideline	Negative (With metabolic activation)
A.	Bacterial Test (Gene mutation)			Negative (Without metabolic activation)
B.	Non-Bacterial In Vitro Test (Chromosomal aberrations)	CHL cells	OECD Guideline No.473 and Japanese Guidelines	Positive (With metabolic activation) Negative (Without metabolic activation)
5.6	Genetic Toxicity In Vivo	Mouse	Unknown	Positive (detailed data are not clear)
5.8	Toxicity to Reproduction	Rat	OECD Preliminary Reproductive Toxicity Test	NOEL Parental = 300 mg/kg/day NOEL F1 offspring = 300 mg/kg/day
5.9	Developmental Toxicity/ Teratogenicity			
5.11	Experience with Human Exposure			

#### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type of test: static ; semi-static ; flow-through ; other   
open-system ; closed-system

Species: *Oryzias latipes*

Exposure period: 96 hr

Results: LC<sub>50</sub> (24h) = 11 mg/l (95% confidence level: 3.3-36 mg/l)  
LC<sub>50</sub> (48h) = 9.8 mg/l (95% confidence level: 5.8-16 mg/l)  
LC<sub>50</sub> (72h) = 9.8 mg/l (95% confidence level: 5.8-16 mg/l)  
LC<sub>50</sub> (96h) = 9.8 mg/l (95% confidence level: 5.8-16 mg/l)  
NOEC =  
LOEC =

Analytical monitoring: Yes  No  ?

Method: OECD Test Guideline 203 (1984)

GLP: Yes  No  ?

Test substance: 3-Methyl-4-nitrophenol, purity = > 98 %

Remarks: A group of 10 fishes were exposed to 5 nominal concentrations (1.8-18 mg/l) and laboratory water control.

Reference: EA, Japan (1992) (HPV/SIDS Test conducted by EA)

(b)

Type of test: static ; semi-static ; flow-through ; other ;  
open-system  closed-system

Species: *Oryzias latipes*

Exposure period: 48 hrs

Results: LC<sub>50</sub> (48h) = 8.4 mg/l

Analytical monitoring: Yes  No  ?

Method:

GLP: Yes  No  ?

Remarks:

Reference: Miyamoto, J. et al. (1978)

#### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

##### A. *Daphnia*

(a)

Type of test: static ; semi-static ; flow-through ; other ;  
open-system ; closed-system

Species: *Daphnia magna*

Exposure period: 24 hrs

Results: EC<sub>50</sub> (24h) = 9.1 mg/l (95% confidence level: 7.9-11 mg/l)  
EC<sub>50</sub> (48h) =  
NOEC =  
LOEC =

Analytical monitoring: Yes  No  ?

Method: OECD Test Guideline 202 (1984)

GLP: Yes  No  ?

Test substance: 3-Methyl-4-nitrophenol, purity = > 98 %

Remarks: 20 daphnids (4 replicates; 5 organisms per replicate) were exposed To 5 nominal concentrations (3.2-32 mg/l) and laboratory water control.

Reference: EA, Japan (1992)

(b)  
Type of test: static []; semi-static []; flow-through [];  
other [];  
open-system []; closed-system []  
Species: *Daphnia magna*  
Exposure period: 24 hrs  
Results: EC<sub>50</sub>(24h) = 33 mg/l  
EC<sub>50</sub>(48h) =  
EC<sub>0</sub>(24h) = 18 mg/l  
EC<sub>100</sub>(24h) = 50 mg/l  
EC<sub>0</sub>(48h) =  
Analytical monitoring: Yes [] No [] ? []  
Method: Method according to Bringmann & Kuhn  
GLP: Yes [] No [] ? []  
Remarks:  
Reference: Bringmann, G. & Kuhn, R. (1977b)

(c)  
Type of test: static []; semi-static []; flow-through []; other [];  
open-system []; closed-system []  
Species: *Daphnia magna*  
Exposure period: 24 hrs  
Results: EC<sub>50</sub>(24h) = 7.8 mg/l  
EC<sub>50</sub>(48h) =  
EC<sub>0</sub>(24h) = 4.5 mg/l  
EC<sub>100</sub>(24h) = 16 mg/l  
Analytical monitoring: Yes [] No [] ? []  
Method: Standard method DIN 38412 Part II (draft)  
GLP: Yes [] No [] ? []  
Remarks:  
Reference: Bringmann, G. & Kuhn, R. (1982)

## B. OTHER AQUATIC ORGANISMS

(a)  
Type of test: static []; semi-static []; flow-through []; other [];  
open-system []; closed-system []  
Species: *Crangon septemspinosa* (sand shrimp)  
Exposure period:  
Results: LC<sub>50</sub>(96h) = 6.8 mg/l  
NOEC =  
LOEC =  
Analytical monitoring: Yes [] No [] ? []  
Method:  
GLP: Yes [] No [] ? []  
Test substance: 3-Methyl-4-nitrophenol  
Remarks:  
Reference: Mcleese, D.W. et al. (1979)

(b)  
Type of test: static []; semi-static []; flow-through []; other [];  
open-system []; closed-system []

Species: *Procambarus clarkii* (Red Swamp Crayfish)  
 Exposure period: 48 hrs (Renewal at 24 hrs)  
 Results: NOEC = 400 mg/l  
 Analytical monitoring: Yes  No  ?   
 Method:  
 GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol  
 Remarks: A range finding test was carried out and resulted that the highest no observable effect concentration was 400 mg/l exposed one male and one female to the chemical for 24 hours at the concentration of 0.1-400 mg/l.  
 Reference: Foster, G.D. & Crosby, D.G. (1986)

4.3 TOXICITY TO AQUATIC PLANTS e.g. Algae

(a)  
 Species: *Selenastrum capricornutum* ATCC 22662  
 End-point: Biomass ; Growth rate ; Other   
 Exposure period: 72 hrs  
 Results: Biomass: EC<sub>50</sub>(72h) = 8.6 mg/l  
 NOEC = 5.8 mg/l (p < 0.05)  
 LOEC =  
 Analytical monitoring: Yes  No  ?   
 Method: OECD Test Guideline 201 (1984)  
 open-system ; closed-system   
 GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol, purity = >98%  
 Remarks: The EC<sub>50</sub> values were calculated based on 7 nominal concentrations (0.6-19.0 mg/l) and laboratory water control.  
 Reference: EA, Japan (1992)

(b)  
 Species: *Scenedesmus quadricauda*  
 End-point: Biomass ; Growth rate ; Other   
 Exposure period: 24 hrs  
 Results: PGR (24h) = 7.0 mg/l  
 NOEC =  
 LOEC =  
 Analytical monitoring: Yes  No  ?   
 Method: open-system ; closed-system   
 GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol  
 Remarks:  
 Reference: Bringmann, G. et al. (1978)

(c)  
 Species: *Scenedesmus quadricauda*  
 End-point: Biomass ; Growth rate ; Other   
 Exposure period: 7 days  
 Results: PGR (7d) = 6.8 mg/l  
 NOEC =  
 LOEC =  
 Analytical monitoring: Yes  No  ?   
 Method: 27 °C, pH 7.0  
 open-system ; closed-system

GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol  
 Remarks:  
 Reference: Bringmann, G. et al. (1980a)

(d)  
 Species: *Chilomonas paramecium*;  
 End-point: Biomass ; Growth rate ; Other   
 Exposure period:  
 Results: PGR (h) = 5.5 mg/l  
 NOEC =  
 LOEC =

Analytical monitoring: Yes  No  ?   
 Method: 20 °C, pH 6.9  
 open-system ; closed-system

GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol  
 Remarks:  
 Reference: Bringmann, G. et al. (1980b)

#### 4.4 TOXICITY TO BACTERIA

Type: Aquatic ; Field ; Soil ; Other   
 Species: *Pseudomonas putida*  
 Exposure period: 16 hrs  
 Results: EC<sub>3</sub> (16hrs) = 6 mg/l  
 Analytical monitoring: Yes  No  ?   
 Method: According to Bringmann & Kuhn  
 GLP: Yes  No  ?   
 Test substance: 3-Methyl-4-nitrophenol  
 Remarks: Effect growth inhibition  
 Reference: Bringmann, G. & Kuhn, R. (1977a)

#### 4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

##### 4.5.1 CHRONIC TOXICITY TO FISH

No studies located

##### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test: static ; semi-static ; flow-through ; other ;  
 open-system ; closed-system   
 Species: *Daphnia magna*  
 End-point: Mortality ; Reproduction rate ; Other   
 Exposure period: 21 day  
 Results:  
 Mortality:  
 LC<sub>50</sub> (24 h) = 19 mg/l (95% confidence level: 12-71 mg/l)  
 LC<sub>50</sub> (48 h) = 12 mg/l (95% confidence level: 8.6-26 mg/l)  
 LC<sub>50</sub> (96 h) = 5.6 mg/l (95% confidence level: 4.7-7.0 mg/l)  
 LC<sub>50</sub> (7 d) = 4.4 mg/l (95% confidence level: 3.7-5.2 mg/l)  
 LC<sub>50</sub> (14 d) = 4.1 mg/l (95% confidence level: 3.5-4.9 mg/l)  
 LC<sub>50</sub> (21 d) = 2.9 mg/l (95% confidence level: 2.4-3.5 mg/l)  
 NOEC  
 LOEC  
 Reproduction:  
 EC<sub>50</sub> (14 d) = 4.1 mg/l (95% confidence level: 3.5-4.7 mg/l)

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EC<sub>50</sub> (21 d) = 3.9 mg/l (95% confidence level: 3.6-4.3 mg/l)  
NOEC = 0.78 mg/l (p < 0.05)  
LOEC = 2.5 mg/l (p < 0.05)  
Analytical monitoring: Yes  No  ?   
Method: OECD Test Guideline 202 (1984)  
GLP: Yes  No  ?   
Test substance: 3-Methyl-4-nitrophenol; Purity > 98 %  
Remarks: 40 daphnids (4 replicates; 10 organisms per replicate) were exposed to 5 nominal concentration (1-10 mg/l) and laboratory water control.  
Reference: EA, Japan (1992)

**4.6 TOXICITY TO TERRESTRIAL ORGANISMS**

**4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS**

No studies located

**4.6.2 TOXICITY TO TERRESTRIAL PLANTS**

No studies located

**4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)**

No studies located

**4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)**

No studies located

**4.8 BIOTRANSFORMATION AND KINETICS IN ENVIRONMENTAL SPECIES**

No studies located

**4.9 ADDITIONAL REMARKS**

No studies located

## 要 旨

### 試験委託者

環境省

### 表 題

2, 3, 4, 6-テトラクロロフェノールの藻類 (*Selenastrum capricornutum*) に対する生長阻害試験

### 試験番号

A000462-1G

### 試験方法

本試験は、OECD 化学品テストガイドライン No. 201「藻類生長阻害試験」(1984年)に準拠して実施した。

- 1) 被験物質: 2, 3, 4, 6-テトラクロロフェノール
- 2) 暴露方式: 止水式(密閉), 振とう培養(100rpm)
- 3) 供試生物: *Selenastrum capricornutum* (ATCC22662)
- 4) 暴露期間: 72時間
- 5) 試験濃度(設定値):  
対照区, 助剤対照区,  
0.100, 0.225, 0.464, 1.00, 2.15, 4.64, 10.0 mg/L  
(公比: 約2.2)  
助剤濃度一定: 100mg/L (ジメチルホルムアミド使用)
- 6) 試験液量: 100 mL (OECD培地) / 容器
- 7) 連数: 3 容器 / 試験区
- 8) 初期細胞濃度:  $1 \times 10^4$  cells/mL
- 9) 試験温度:  $23 \pm 2$  °C
- 10) 照明: 4000 lux (±20%の変動内, フラスコ液面付近) で連続照明
- 11) 分析法: 高速液体クロマトグラフィー (HPLC)

## 結 果

### 1) 試験液中の被験物質濃度

試験液の分析の結果、暴露開始時の測定値の設定値に対する割合が±20%以内であったため、下記の阻害濃度の算出には設定値を用いた。

### 2) 生長曲線下面積の比較による阻害濃度

50%生長阻害濃度 EbC50 (0-72) : 2.61 mg/L (95%信頼区間 : 算出不可)

最大無作用濃度 NOECb (0-72) : 1.00 mg/L

### 3) 生長速度の比較による阻害濃度

50%生長阻害濃度 ErC50 (24-48) : 3.24 mg/L (95%信頼区間 : 算出不可)

最大無作用濃度 NOECr (24-48) : 2.15 mg/L

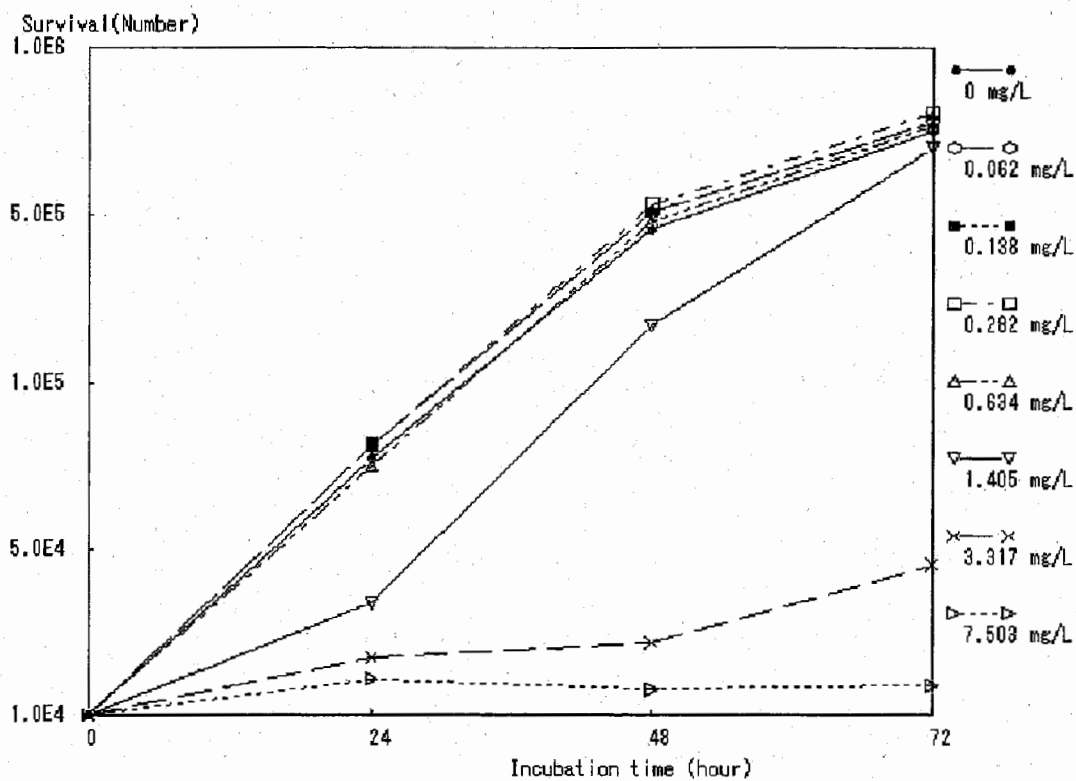
50%生長阻害濃度 ErC50 (24-72) : 3.68 mg/L (95%信頼区間 : 算出不可)

最大無作用濃度 NOECr (24-72) : 2.15 mg/L



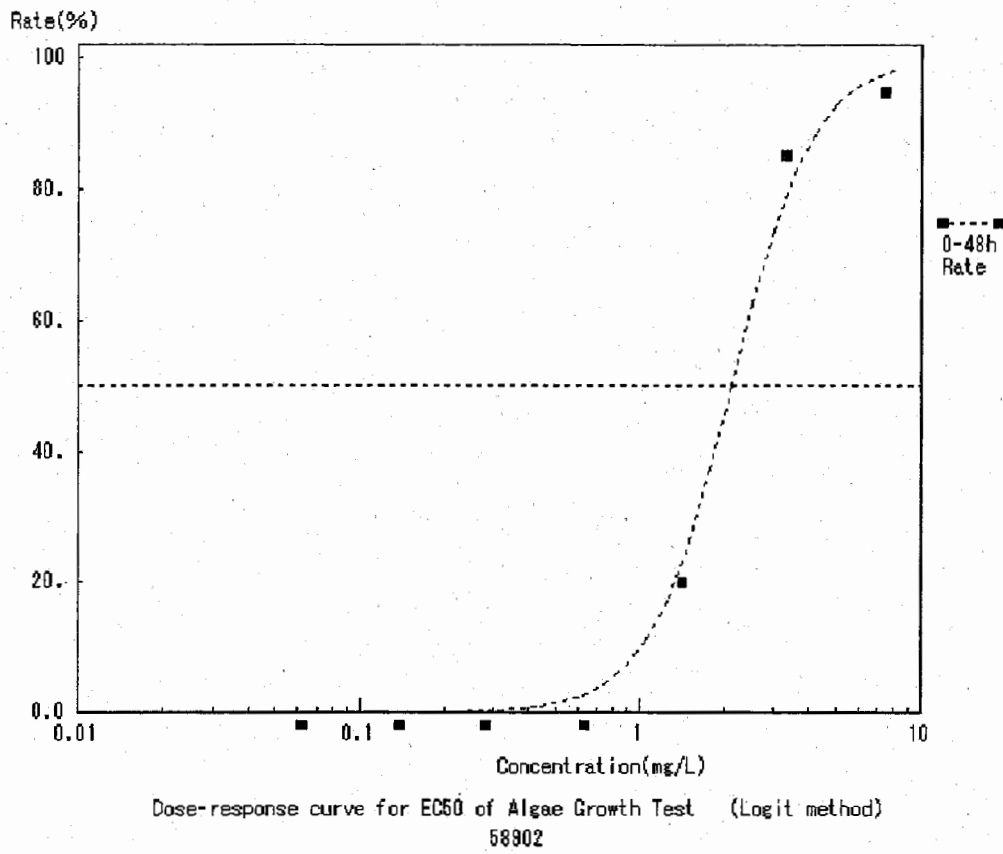
2,3,4,6-テトラクロロフェノール(CAS.58-90-2)

① 生長曲線



Time course pattern of Algae Growth Test  
58902

② 阻害率曲線



③ 毒性値

0-72hErC50 (実測値に基づく) = 2.1mg/L  
0-72hNOECr (実測値に基づく) = 0.63mg/L

## 要 旨

### 試験委託者

環境省

### 表 題

2, 3, 4, 6-テトラクロロフェノールのオオミジンコ (*Daphnia magna*) に対する急性遊泳阻害試験

### 試験番号

A 0 0 0 4 6 2 - 2 G

### 試験方法

本試験は、OECD 化学品テストガイドライン No. 202 「ミジンコ類、急性遊泳阻害試験および繁殖試験」(1984年) に準拠して実施した。

- 1) 被験物質： 2, 3, 4, 6-テトラクロロフェノール
- 2) 暴露方式： 止水式，水面をテフロンシートで被覆
- 3) 供試生物： オオミジンコ (*Daphnia magna*)
- 4) 暴露期間： 48時間
- 5) 試験濃度 (設定値) :  
対照区，助剤対照区，0. 200, 0. 420, 0. 890, 1. 90, 4. 00 mg/L  
公比：約 2. 1  
助剤濃度一定：40 mg/L (ジメチルホルムアミド 使用)
- 6) 試験液量： 100 mL/容器
- 7) 連数： 4 容器/試験区
- 8) 供試生物数： 20頭/試験区 (5頭/容器)
- 9) 試験温度： 20±1℃
- 10) 照明： 16時間明/8時間暗
- 11) 分析法： 高速液体クロマトグラフィー (HPLC)

## 結 果

### 1) 試験液中の被験物質濃度

試験液の分析の結果、測定値の設定値に対する割合が全て±20%以内であったため、結果の算出には設定値を用いた。

### 2) 24 時間暴露後の結果

半数遊泳阻害濃度 (EiC50) : 2.48 mg/L (95%信頼区間 : 2.07~3.11 mg/L)

最大無作用濃度 (NOECi) : 0.420 mg/L

100%阻害最低濃度 : 4.00 mg/L

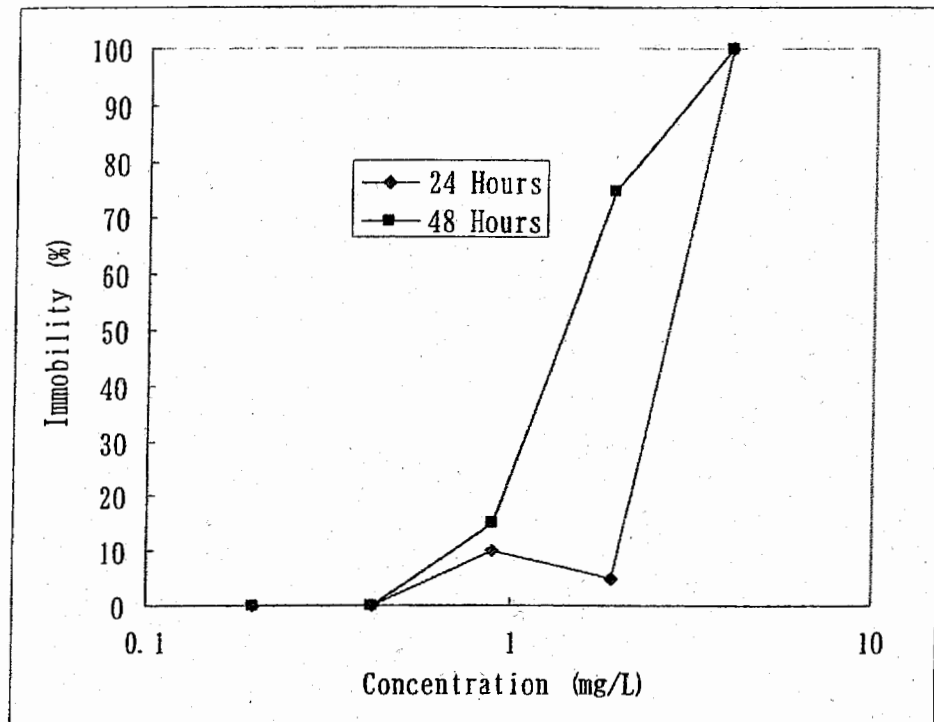
### 3) 48 時間暴露後の結果

半数遊泳阻害濃度 (EiC50) : 1.40 mg/L (95%信頼区間 : 1.15~1.71 mg/L)

最大無作用濃度 (NOECi) : 0.420 mg/L

100%阻害最低濃度 : 4.00 mg/L

Figure 1. Concentration-Response (Immobilty) Curve



## 要 旨

### 試験委託者

環境省

### 表 題

2, 3, 4, 6-テトラクロロフェノールのオオミジンコ (*Daphnia magna*) に対する繁殖阻害試験

### 試験番号

A000462-3G

### 試験方法

本試験は、OECD 化学品テストガイドラインNo. 211「オオミジンコ繁殖試験」(1998年)に準拠して実施した。

- 1) 被験物質： 2, 3, 4, 6-テトラクロロフェノール
- 2) 暴露方式： 半止水式 (2日毎に試験液の全量を交換)  
水面をテフロンシートで被覆
- 3) 供試生物： オオミジンコ (*Daphnia magna*)
- 4) 暴露期間： 21日間
- 5) 試験濃度 (設定値) :  
対照区, 助剤対照区, 0.0200, 0.0600, 0.180, 0.500, 1.50 mg/L  
公比：約 2.9  
助剤濃度一定：75 mg/L (ジメチルホルムアミド 使用)
- 6) 試験液量： 80 mL/容器
- 7) 連数： 10容器/試験区
- 8) 供試生物数：10頭/試験区 (1頭/容器)
- 9) 試験温度： 20±1℃
- 10) 照明： 16時間明/8時間暗
- 11) 分析法： 高速液体クロマトグラフィー (HPLC)

## 結 果

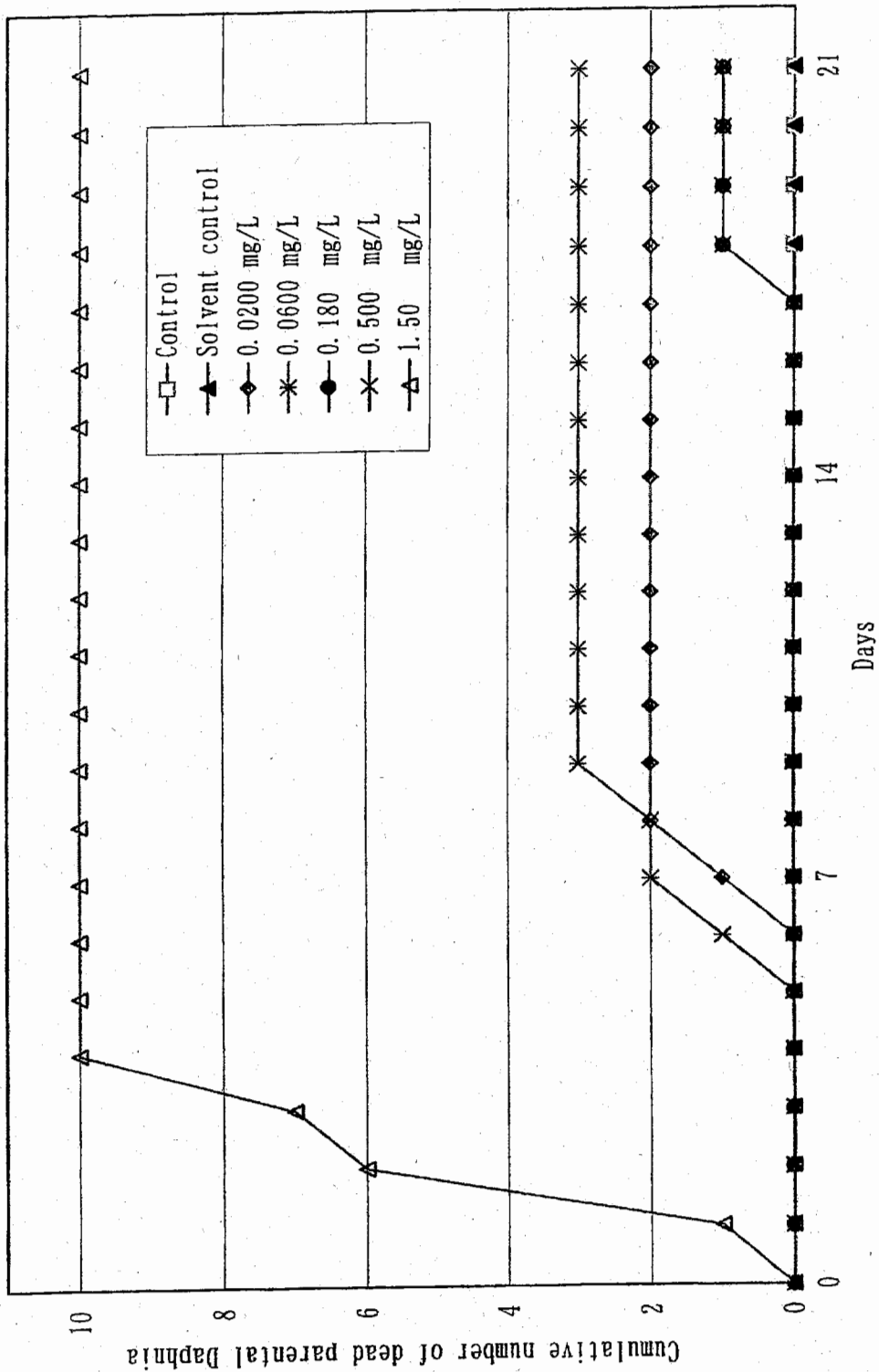
### 1) 試験液中の被験物質濃度

試験液の分析の結果、測定値の設定値に対する割合が、全て±20%以内であったため、結果の算出には設定値を用いた。

### 2) 21日間暴露後の結果

親ミジンコの半数致死濃度 (LC50) :	0.693 mg/L
	(95%信頼区間 : 0.475~1.14 mg/L)
50%繁殖阻害濃度 (EC50) :	0.430 mg/L
	(95%信頼区間 : 0.387~0.466 mg/L)
最大無作用濃度 (NOEC) :	0.180 mg/L
最小作用濃度 (LOEC) :	0.500 mg/L

Figure 1 Cumulative Numbers of Dead Parental *Daphnia*



Values in legend are given in the nominal concentration.

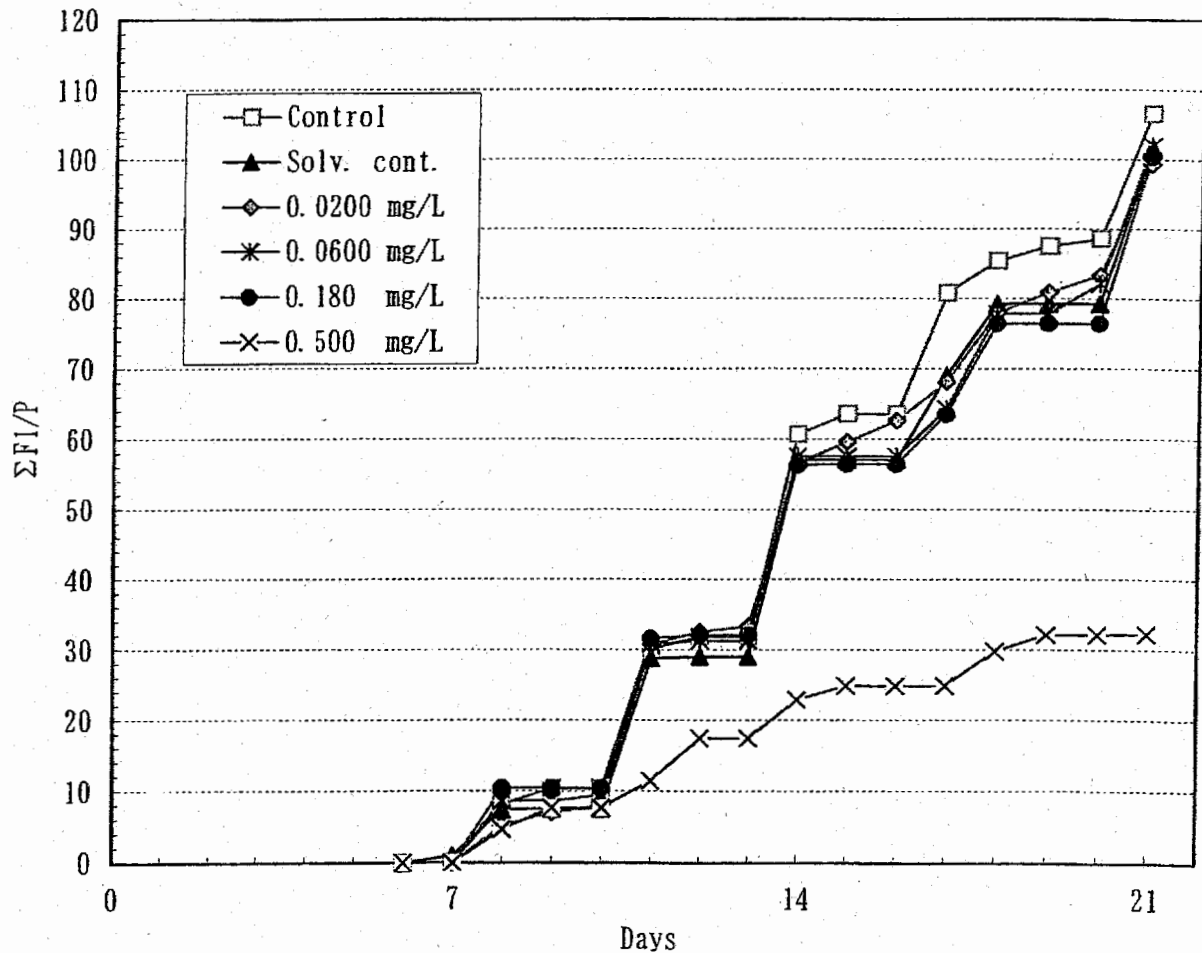


Table 4 Mean Cumulative Numbers of Juveniles Produced per Adult Alive for 21 Days ( $\Sigma F1/P$ )

Nominal Conc.	Days															
	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Control	0.0	0.0	8.1	10.4	10.4	30.1	31.9	31.9	60.7	63.6	63.6	80.8	85.4	87.5	88.6	106.6
Solv. cont.	0.0	1.0	7.4	7.5	7.5	28.8	29.0	29.0	57.1	57.1	57.1	69.1	79.3	79.3	79.3	101.7
0.0200 mg/L	0.0	0.0	5.1	7.0	8.0	30.8	32.6	33.4	56.6	59.6	62.6	68.1	78.0	80.9	83.4	99.4
0.0600 mg/L	0.0	0.0	8.6	8.6	9.4	30.9	31.3	31.3	57.6	57.6	57.6	64.3	77.9	77.9	82.1	102.0
0.180 mg/L	0.0	0.0	10.4	10.4	10.4	31.7	32.1	32.1	56.3	56.4	56.4	63.6	76.4	76.4	76.4	100.4
0.500 mg/L	0.0	0.0	4.7	7.7	7.7	11.4	17.4	17.4	22.9	24.9	24.9	24.9	29.8	32.1	32.1	32.2
1.50 mg/L	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

-: All parental *Daphnia* were dead during a 21-days testing period.

Figure 2 Time Course of  $\Sigma F1/P$  for Each Concentration Level



Values in legend are given in the nominal concentration.

## 要 旨

### 試験委託者

環境省

### 表 題

2, 3, 4, 6-テトラクロロフェノールのヒメダカ (*Oryzias latipes*) に対する急性毒性試験

### 試験番号

A 0 0 0 4 6 2 - 4 G

### 試験方法

本試験は、OECD 化学品テストガイドライン No. 203 「魚類毒性試験」 (1992年) に準拠して実施した。

- 1) 被験物質： 2, 3, 4, 6-テトラクロロフェノール
- 2) 暴露方式： 半止水式 (24時間毎に試験液の全量を交換), 水面をテフロンシートで被覆
- 3) 供試生物： ヒメダカ (*Oryzias latipes*)
- 4) 暴露期間： 96時間
- 5) 試験濃度 (設定値) : 対照区, 助剤対照区, 0. 200, 0. 360, 0. 630, 1. 10, 2. 00 mg/L  
公比 : 約1. 8  
最高助剤濃度 : 20. 0 mg/L (ジメチルホルムアミド使用)
- 6) 試験液量 : 5. 0 L / 容器
- 7) 連数 : 1 容器 / 試験区
- 8) 供試生物数 : 10尾 / 試験区
- 9) 試験温度 : 24 ± 1 °C
- 10) 照明 : 室内光, 16時間明 / 8時間暗
- 11) 分析法 : 高速液体クロマトグラフィー (HPLC)

### 結 果

- 1) 試験液中の被験物質濃度 : 試験液の分析の結果, 測定値の設定値に対する割合が, ±20% を超える値があったため, 結果の算出には測定値の幾何平均値を用いた。
- 2) 96 時間の半数致死濃度 (LC50) : 0. 557 mg/L  
(95%信頼区間 : 0. 403 mg/L ~ 0. 774 mg/L)

Figure 1 Concentration-Mortality Curve

