Chemical Name ; Methyl dichloroacetate

Synonym ; Dichloro acetic acid methyl ester

Molecular Weight ; 142.97
Melting Point ; -52℃[Aldrich]
Boiling Point ; 143℃[Aldrich]
Flashing Point ; 80℃[Aldrich]
Molecular Formula ; $C_3H_4Cl_2O_2$

Chemical Structure

$Cl_2CHCOOCH_3$

CAS No. ; 116-54-1
MITI No. ; (2)-1163
ML No. ; －
Specified Chemical Substances ; －

Source of Substance; Aldrich
Lot No. ; 07609KW
Purity ; >99%

Vehicle ; DMSO

Judgement for
Chromosomal Aberration in CHL ; Positive

IARC Evaluation ; not yet cited

Treatment			No. of Metaphase	Polyploid		Cell with Structural Chromosome Aberration (%)								
Substance	Time (h)	Concentration (mg/ml)		(%)	Judgement	Gap	Chromatid		Chromosome		Others	Total		Judgement
						g	ctb	cte	csb	cse		－g	＋g	
DMSO	24	1.0%	200	0	－	0	1	0	0	0	0	1	1	－
	48	1.0%	200	0	－	0	0	0	0	0	0	0	0	－
Test Chemical	24	0.8	200	0.5	－	0.5	2	0.5	0	0	0	2.5	2.5	－
		1.2	200	0.5	－	0	2	0	0	0	0	2	2	－
		1.6	200	2	－	1	1.5	3	0	0	0	4.5	4.5	－
		2.0	200	2	－	0	4.5	4.5	0	0	0	7	7	±
		2.4	200	1	－	0	30.5	45	0	0	0	54.5	54.5	＋
	48	0.8	200	0.5	－	0	0	2	0	0	0	2	2	－
		1.2	200	1.5	－	0	0.5	0	0	0	0	0.5	0.5	－
		1.6	200	0.5	－	0	2	2	0	0	0	3	3	－
		2.0	200	1	－	0	1	4	0	0	0	5	5	±
		2.4	200	2	－	1	10	10	0	0.5	0	17.5	18.5	＋
Positive Control [MMC]	24	0.00004	200	0	－	0.5	20	35	0	0	0	47	47.5	＋
	48	0.00004	200	0.5	－	0	21	57	0	0	0	62	62	＋

※ The precipitation of test chemical was observed in the cultre medium over 1.6mg/ml.

Experimental Data with Metabolic Activation

Treatment			No. of Metaphase	Polyploid		Cell with Structural Chromosome Aberration (%)								
Substance	S9 mix	Concent-ration (mg/ml)		(%)	Judge-ment	Gap	Chromatid		Chromosome		Others	Total		Judge-ment
						g	ctb	cte	csb	cse		−g	+g	
DMSO	−	1.0%	200	0	−	0	0.5	0	0	0	0	0.5	0.5	−
	+	1.0%	200	0.5	−	0	0	0	0	0	0	0	0	−
Test Chemical	−	0.25	200	1	−	0	0	0	0	0	0	0	0	−
		0.5	200	1	−	0	0.5	0.5	0	0	0	1	1	−
		1.0	200	0.5	−	0	0	1.5	0	0	0	1.5	1.5	−
		2.0	200	0.5	−	0	1	0.5	0	0	0	1	1	−
		4.0	No obserbation for metaphase											
	+	0.25	200	0.5	−	0	0	0	0	0	0	0	0	−
		0.5	200	7.5	±	0	0	3.5	0	0	0	3.5	3.5	−
		1.0	200	2	−	0	10.5	39	0	0.5	0	40	40	+
		2.0	162	1.2	−	0.6	45.7	87.7	0	0	0	89.5	89.5	+
		4.0	No obserbation for metaphase											
Positive Control [B[a]P]	−	0.01	200	0	−	0	0.5	0.5	0.5	0	0	1.5	1.5	−
	+	0.01	200	0	−	0	2	20	0	0	0	21.5	21.5	+

※ Test conditions: Treatment time ; 6h, Rcovery time ; 18h

※ The precipitation of test chemical was observed in the cultre medium over 2.0mg/ml.