TABLE 52

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO LOW CONCENTRATION PRIME URETHANE "B" TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	3.7	---
N,N-Dimethylacrylamide	3 - 15	6.2	---
1,2,3-Trichloropropane	1 - 5	4.6	2.4
N,N-Dimethylformamide	0.5 - 2	0.7	---
N,N-Dimethylacetamide	0.5 - 2	0.6	---
Octamethylcyclotetrasiloxane	1 - 5	4.1	---
1,3-Dichloro-2-propanol	1 - 5	2.7	13.5
Other (listed below)	---	1.0 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Methanonaphthalene, (Chloromethyl)Oxirane.

TABLE 53

SUMMARY EXPOSURE DATA FOR SPONGE RUBBER SYNTHESIZED MIXTURES

Exposure Conditions	Exposure Date	Maximum Respiratory Depression (% below Baseline)	Average Exposure Concentration (ppm as propane)	Precision of Exposure Concentration (%RSD)
Test Mixture	09/01/95	41.9	35.8	4.8
Test Mixture without 2-Methylnaphathalene	09/08/95	17.0	24.0	15.7
Test Mixture without 2-Methylnaphathalene or 1,4-Dimethylnaphathalene	10/09/95	4.2*	31.9	5.6
Low concentration Test Mixture (A)	10/17/95	36.2	17.5	8.4
Lower concentration Test Mixture (B)	11/01/95	14.7	9.0	10.3
Lowest concentration Test Mixture (C)	11/28/95	9.8*	5.8	10.7

*Respiratory depression not considered significant.

TABLE 54

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO SPONGE RUBBER TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.1 - 0.5	0.3	---
N,N-Dimethylacetamide	0.5 - 2	1.1	---
Toluene	0.2 - 1	1.0	---
Undecane	5 - 20	9.3	---
1,2,4-Trimethylbenzene	5 - 20	13.9	---
2-Methylnaphthalene	2 - 8	11.5	60.3
1,4-Dimethylnaphthalene	5 - 20	8.1	---
Diphenyl ether	0.5 - 2	2.4	---
Other (listed below)	---	0.2 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 2-Ethyltoluene, Butyl benzene.

TABLE 55

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO SPONGE RUBBER TEST MIXTURE WITH 2-METHYLNAPHTHALENE REMOVED

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.1 - 0.5	0.5	---
N,N-Dimethylacetamide	0.5 - 2	1.6	---
Toluene	0.2 - 1	1.3	---
Undecane	5 - 20	10.2	---
1,2,4-Trimethylbenzene	5 - 20	16.2	---
2-Methylnaphthalene	0	0.3	---
1,4-Dimethylnaphthalene	5 - 20	4.5	---
Diphenyl ether	0.5 - 2	1.4	---
Other (listed below)	---	0.2 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 2-Ethyltoluene, 1-Methylpropylbenzene, Butyl benzene.

TABLE 56

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO SPONGE RUBBER TEST MIXTURE WITH 2-METHYLNAPHTHALENE AND 1,4-DIMETHYLNAPHTHALENE REMOVED

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.1 - 0.5	nd	---
N,N-Dimethylacetamide	0.5 - 2	0.2	---
Toluene	0.2 - 1	1.1	---
Undecane	5 - 20	11.1	---
1,2,4-Trimethylbenzene	5 - 20	15.1	---
2-Methylnaphthalene	0	nd	---
1,4-Dimethylnaphthalene	0	nd	---
Diphenyl ether	0.5 - 2	1.1	---
Other (listed below)	---	0.1 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 2-Ethyltoluene.

TABLE 57

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO LOW CONCENTRATION SPONGE RUBBER TEST MIXTURE (A)

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.1 - 0.5	nd	---
N,N-Dimethylacetamide	0.5 - 2	nd	---
Toluene	0.2 - 1	0.4	---
Undecane	5 - 20	5.4	---
1,2,4-Trimethylbenzene	5 - 20	8.0	---
2-Methylnaphthalene	2 - 8	5.1	39.0
1,4-Dimethylnaphthalene	5 - 20	7.3	---
Diphenyl ether	0.5 - 2	1.1	---
Other (listed below)	—	0.2 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 2-Ethyltoluene, 1-Methylnaphthalene.

TABLE 58

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO LOWER CONCENTRATION SPONGE RUBBER TEST MIXTURE (B)

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.05 - 0.1	0.1	---
N,N-Dimethylacetamide	0.2 - 0.4	0.3	---
Toluene	0.1 - 0.2	0.3	---
Undecane	2 - 5	3.4	---
1,2,4-Trimethylbenzene	2 - 5	5.6	---
2-Methylnaphthalene	1 - 2	1.9	13.1
1,4-Dimethylnaphthalene	2 - 4	1.4	---
Diphenyl ether	0.2 - 0.5	0.4	---
Other (listed below)	---	0.2 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 1-Methylnaphthalene, 2-Ethyltoluene, 1-Undecene, BHT, Isooctane, Benzene.

TABLE 59

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO LOWEST CONCENTRATION SPONGE RUBBER TEST MIXTURE (C)

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
N,N-Dimethylformamide	0.03 - 0.05	0.8	---
N,N-Dimethylacetamide	0.1 - 0.2	0.5	---
Toluene	0.05 - 0.1	0.1	---
Undecane	1 - 3	1.8	---
1,2,4-Trimethylbenzene	1 - 3	3.2	---
2-Methylnaphthalene	0.5 - 1	1.0	---
1,4-Dimethylnaphthalene	1 - 2	1.1	---
Diphenyl ether	0.1 - 0.3	0.2	---
Other (listed below)	---	0.03 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Trichlorofluoromethane, Octamethylcyclotetrasiloxane.

TABLE 60

SUMMARY EXPOSURE DATA FOR BONDED URETHANE SYNTHESIZED MIXTURES

Exposure Conditions	Exposure Date	Maximum Respiratory Depression (% below Baseline)	Average Exposure Concentration (ppm as propane)	Precision of Exposure Concentration (%RSD)
Test Mixture	10/03/95	36.3	41.4	7.6
Test Mixture without BHT	10/06/95	4.7*	44.0	16.0
Low concentration Test Mixture	10/31/95	7.4*	18.3	10.5

*Respiratory depression not considered significant.

TABLE 61

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO BONDED URETHANE TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	5.9	16.1
Adiponitrile	0.2 - 1.0	1.6	---
Undecene+Tridecene	10 - 50	22.4 (15.0 + 7.4)	---
Decane	0.5 - 2	1.8	---
N,N-Dimethylacetamide	5 - 20	9.3	---
TXIB	0.5 - 2	1.0	---
Other (listed below)	--	3.0 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Substituted methanonaphthalene, 1,3,3-Trimethylbicyclo[2.2.1]heptane, 4-PCH, 1-Decene

TABLE 62

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO BONDED URETHANE TEST MIXTURE WITH BHT REMOVED

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	0	nd	---
Adiponitrile	0.2 - 1.0	2.3	---
Undecene+Tridecene	10 - 50	39.1 (20.3 + 18.8)	---
Decane	0.5 - 2	2.1	---
N,N-Dimethylacetamide	5 - 20	8.3	---
TXIB	0.5 - 2	4.2	---
Other (listed below)	--	0.3 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 2,3-Dimethyl-1,4-hexadiene, 1-Dodecyne, Ethyl acetate, c-1,5-Heptadiene, 1-Dodecene

TABLE 63

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO LOW CONCENTRATION BONDED URETHANE TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	5.4	11.6
Adiponitrile	0.2 - 1.0	nd	---
Undecene+Tridecene	10 - 50	15.4 (10.1 + 5.3)	---
Decane	0.5 - 2	1.0	---
N,N-Dimethylacetamide	5 - 20	1.9	---
TXIB	0.5 - 2	0.2	---
Other (listed below)	--	0.5 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Substituted methanonaphthalene, Norflurane, Ether, Isooctane, Benzene.

TABLE 64

SUMMARY EXPOSURE DATA FOR SBR CARPET SYNTHESIZED MIXTURES

Exposure Conditions	Exposure Date	Maximum Respiratory Depression (% below Baseline)	Average Exposure Concentration (ppm as propane)	Precision of Exposure Concentration (%RSD)
Test Mixture	10/11/95	8.0*	28.8	15.7
Test Mixture with Decanol	10/30/95	7.2*	38.4	5.9

*Respiratory depression not considered significant.

TABLE 65

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO SBR CARPET TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
4-PCH	1 - 5	8.0	---
4-VCH	0.5 - 2	2.4	---
Styrene	1 - 5	6.3	---
Toluene	2 - 10	10.7	---
Isooctane	0.5 - 2	2.1	---
Acetic acid	2 - 10	1.2	---
Propylbenzene	0.5 - 2	2.7	---
Dodecanol	1 - 5	nd	---
Cyclohexanol	1 - 5	4.9	---
Undecane	1 - 5	6.8	---
Other (listed below)	---	0.3 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 3-ethenyl-4-(1-methylethenyl)cyclohexene, octamethylcyclotetrasiloxane, cyclohexene.

TABLE 66

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO SBR CARPET TEST MIXTURE WITH DECANOL

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
4-PCH	1 - 5	8.3	---
4-VCH	0.5 - 2	2.1	---
Styrene	1 - 5	5.5	---
Toluene	2 - 10	9.2	---
Isooctane	0.5 - 2	1.9	---
Acetic acid	2 - 10	0.2	---
Propylbenzene	0.5 - 2	2.8	---
Decanol	1 - 5	4.2	---
Cyclohexanol	1 - 5	5.1	---
Undecane	1 - 5	6.5	---
Other (listed below)	---	0.2 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Substituted Bicyclo[2.2.1] heptanes, BHT, Undecene.

TABLE 67

SUMMARY EXPOSURE DATA FOR COMPLAINT SYSTEM "A" SYNTHESIZED MIXTURES

Exposure Conditions	Exposure Date	Maximum Respiratory Depression (% below Baseline)	Average Exposure Concentration (ppm as propane)	Precision of Exposure Concentration (%RSD)
Test Mixture	10/26/95	18.2	45.8	8.2
Test Mixture (repeat)	11/21/95	19.5	47.9	11.3
Test Mixture without BHT	10/27/95	6.3*	43.1	3.5
Test Mixture without BHT (repeat)	11/10/95	6.6*	34.5	7.1

*Respiratory depression not considered significant.

TABLE 68

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "A" TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	9.5	40.5
Phenol	0.5 - 2	1.8	---
N,N-Dimethylacetamide	0.5 - 2	2.4	---
Nonanal	0.2 - 1	1.1	---
3-Methylcyclohexanol	0.5 - 2	2.8	---
1,2,4-Trimethylbenzene	0.5 - 2	4.6	---
Undecene	5 - 20	24.2	---
Decane	0.5 - 2	4.9	---
o-Hydroxybiphenyl*		3.7	---
Other (listed below)	---	2.1 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 3-Methylhexane, 2-Methylhexane, Heptane, Decamethylcyclopentasiloxane, Ether, Methanonaphthalene, Isooctane.

* o-Hydroxybiphenyl quantified relative to its own response, removed from test mixture due to difficulty in controlling vapor generation.

TABLE 69

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "A" TEST MIXTURE (REPEAT)

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	7.2	26.3
Phenol	0.5 - 2	3.3	---
N,N-Dimethylacetamide	0.5 - 2	2.9	---
Nonanal	0.2 - 1	1.5	---
3-Methylcyclohexanol	0.5 - 2	3.3	---
1,2,4-Trimethylbenzene	0.5 - 2	4.4	---
Undecene	5 - 20	> 18.0*	---
Decane	0.5 - 2	4.7	---
Other (listed below)	---	0.4 (Toluene equivalents)	---

*Concentration estimated, data for this compound were outside of linear range of mass spec.
Other compounds identified (in decreasing order of concentration): 3-Methylhexane, 2-Methylhexane, Heptane, 4-Phenylcyclohexene, 2-Ethyltoluene, 1-Undecyne, Methanonaphthalene.

TABLE 70

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "A" TEST MIXTURE WITH BHT REMOVED

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	0	< 0.1	---
Phenol	0.5 - 2	2.0	---
N,N-Dimethylacetamide	0.5 - 2	2.7	---
Nonanal	0.2 - 1	1.5	---
3-Methylcyclohexanol	0.5 - 2	3.0	---
1,2,4-Trimethylbenzene	0.5 - 2	4.4	---
Undecene	5 - 20	22.1	---
Decane	0.5 - 2	4.5	---
o-Hydroxybiphenyl*	---	0.1	---
Other (listed below)	---	0.7 (Toluene equivalents)	---

* o-Hydroxybiphenyl quantified relative to its own response, removed from test mixture due to difficulty in controlling vapor generation.
Other compounds identified (in decreasing order of concentration): Ether, Isooctane, 5-Undecene, 1-Undecyne, Undecane, 4-Ethyltoluene, 1,1,1-Trichloroethane, Ethyl Acetate, Benzene, 2-Ethyl-1-hexanol, 2-Ethylhexanal, Dibenzofuran, 1,1'-Biphenyl.

TABLE 71

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "A" TEST MIXTURE WITH BHT REMOVED (REPEAT)

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	0	nd	---
Phenol	0.5 - 2	1.5	---
N,N-Dimethylacetamide	0.5 - 2	0.9	---
Nonanal	0.2 - 1	0.4	---
3-Methylcyclohexanol	0.5 - 2	1.7	---
1,2,4-Trimethylbenzene	0.5 - 2	3.9	---
Undecene	5 - 20	17.6	---
Decane	0.5 - 2	4.2	---
Other (listed below)	---	2.4 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Ethyl acetate, Ether, Trichlorofluoromethane, Carbon Disulfide, Chloroform, Dibenzofuran, 1,1'-Biphenyl, 1,1,1,-Trichloroethylene, Isooctane, Benzene, 4-Phenylcyclohexene.

TABLE 72

SUMMARY EXPOSURE DATA FOR COMPLAINT SYSTEM "B" SYNTHESIZED MIXTURES

Exposure Conditions	Exposure Date	Maximum Respiratory Depression (% below Baseline)	Average Exposure Concentration (ppm as propane)	Precision of Exposure Concentration (%RSD)
Test Mixture	10/20/95	26.2	20.4	15.1
Test Mixture without BHT	10/23/95	8.0*	10.5	17.0

*Respiratory depression not considered significant.

TABLE 73

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "B" TEST MIXTURE

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	5 - 20	7.9	31.0
Isobornyl acetate	0.5 - 2	2.8	---
N,N-Dimethylacetamide	0.5 - 2	2.8	---
Undecene	1 - 5	3.2	---
4-Morpholine ethanamine	0.5 - 2	0.2	---
Other (listed below)	---	0.5 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): Camphene, Methanonaphthalene, 6-Isopropylidene-1-methyl-bicyclo[3.1.0]hexane, cis-2-methylene-3-(1-methylethyl)cyclohexanol acetate.

TABLE 74

SUMMARY CONCENTRATION DATA FOR EXPOSURE TO COMPLAINT SYSTEM "B" TEST MIXTURE WITH BHT REMOVED

Compound	Concentration Range (mg/m^3)		Predicted %RD (based on Task 1 data)
	Target	Average Conc. Detected	
BHT	0	0.1	---
Isobornyl acetate	0.5 - 2	2.4	---
N,N-Dimethylacetamide	0.5 - 2	2.7	---
Undecene	1 - 5	4.3	---
4-Morpholine ethanamine	0.5 - 2	1.9	---
Other (listed below)	---	2.1 (Toluene equivalents)	---

Other compounds identified (in decreasing order of concentration): 4-Isobutylmorpholine, Undecane, 1-Octanol, Camphene, 1-methyl-4-(1-methylethylidene)cyclohexene, 1-Dodecene, Morpholine, 2-Methylundecane, Isooctane, 1,7,7-trimethyl-tricyclo[2.2.1.02,6]heptane, Octyl-oxirane.

TABLE 75

QUALITY CONTROL DATA FROM DUPLICATE TASK 1 EXPOSURES

Compound	Exposure Date	Average Exposure Concentration (mg/m^3)	Maximum % Respiratory Depression	% Relative deviation of RD
1,2,3-Trichloropropane	09/15/95	27.0	14.6	19.3
	02/17/95	34.1	21.6	
	02/16/95	59.7	47.7	5.2
	03/06/95	62.1	52.9	
2,6-Di-*tert*-butyl-4-methylphenol (BHT)	04/24/95	7.4	25.4	10.2
	02/07/95	7.4	20.7	
	02/08/95	10.7	50.1	7.2
	01/31/95	10.7	45.5	
	09/15/95	10.9	43.6	
4-Phenylcyclohexene	03/20/95	138	33.8	4.4
	03/20/95	142	36.9	
2-Methylnaphthalene	04/12/95	4.5	29.7	0.7
	06/29/95	4.4	30.1	

TABLE 76

QUALITY CONTROL DATA FROM DUPLICATE TASK 2 EXPOSURES

Mixture	Exposure Date	Average Exposure Concentration (ppm as propane)	Maximum % Respiratory Depression	% Relative mean deviation of RD
Complaint System "A" Test Mixture	10/26/95	45.8	18.2	3.4
	11/21/95	47.9	19.5	
Complaint System "A" without BHT	10/27/95	43.1	6.3*	NA*
	11/10/95	34.5	6.6*	

*Respiratory depression not considered significant.

TABLE 77

SUMMARY EXPOSURE DATA FOR FORMALDEHYDE

Exposure Date	Average Exposure Concentration (mg/m^3)	Precision of Exposure Concentration (%RSD)	Maximum Respiratory Depression (% below Baseline)
03/15/95	2.8	7.1	28.6
03/13/95	5.6	7.4	36.8
03/09/95	6.0	5.6	44.1
03/13/95	8.4	22.7	49.8
03/14/95	16.5	3.3	49.4

CHAPTER 11.0

FIGURES

FIGURE 1

SCHEMATIC OF THE J-TUBE METHOD FOR VAPOR GENERATION

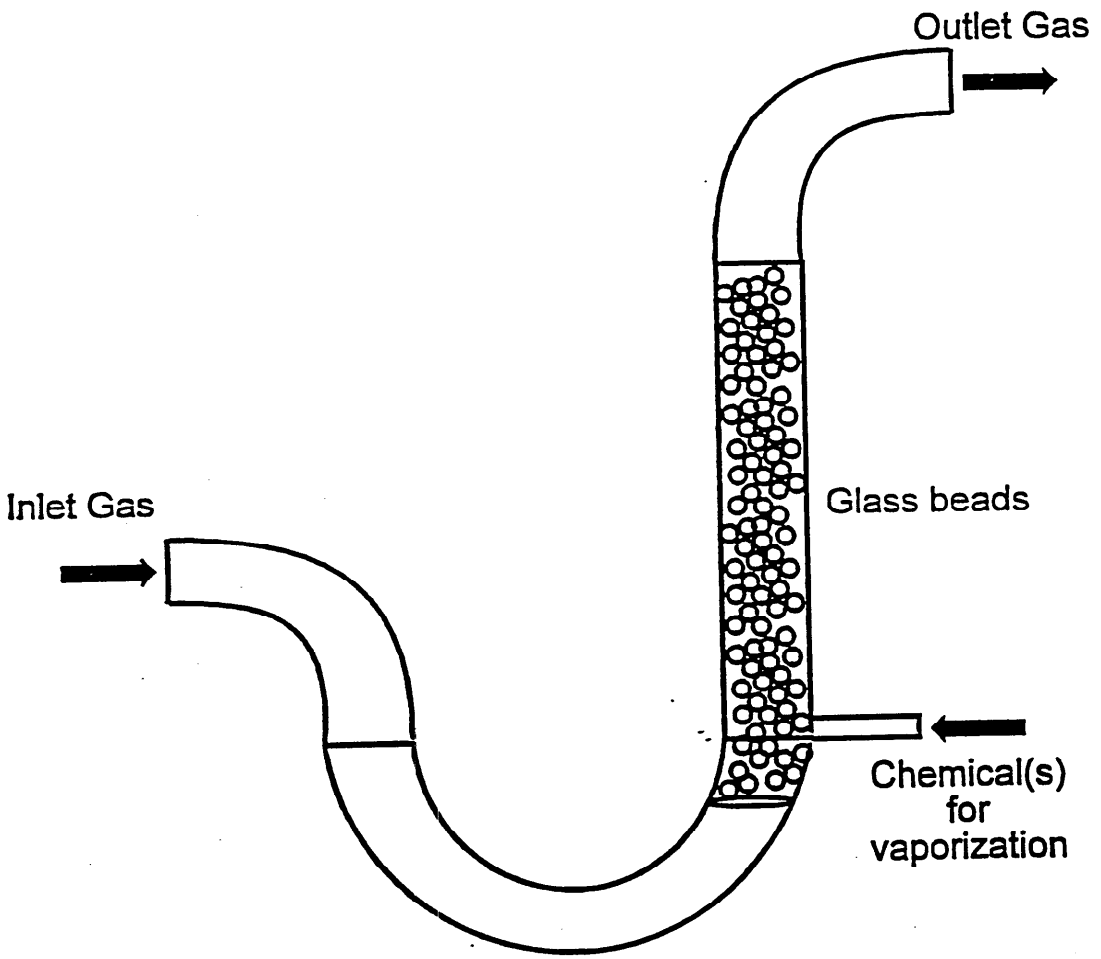


FIGURE 2

SCHEMATIC OF THE FLASK METHOD FOR VAPOR GENERATION

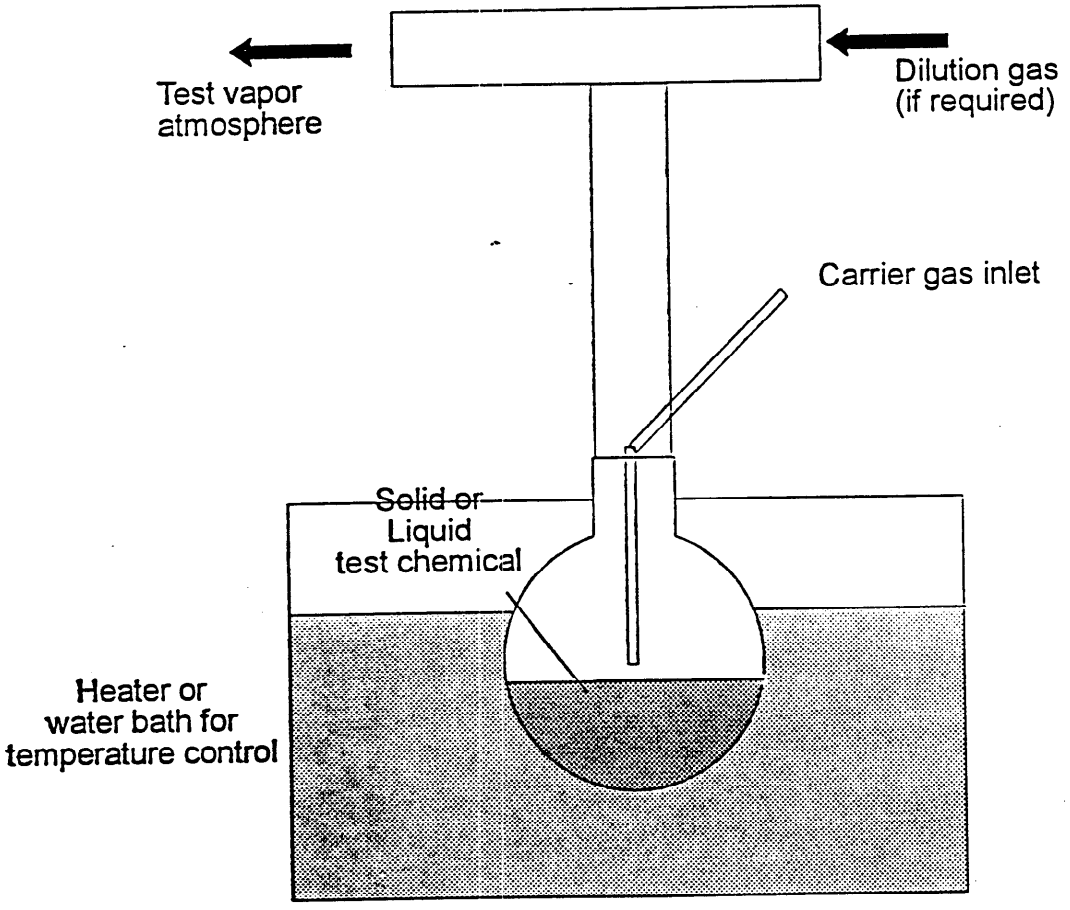


FIGURE 3

THE CHARACTERISTIC WAVEFORMS OF RESPIRATORY IRRITATION

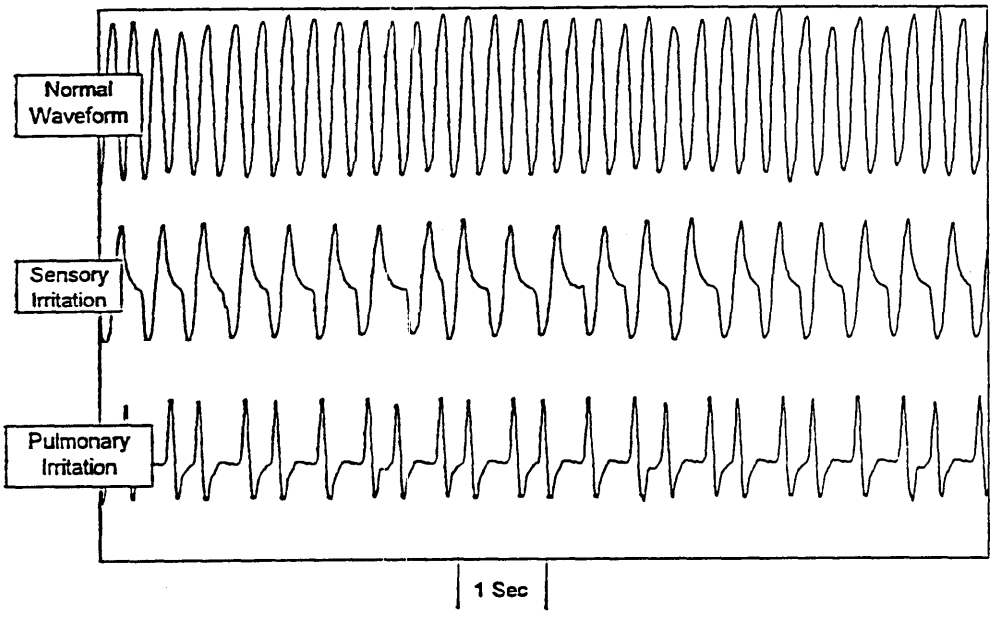


FIGURE 4

SCHEMATIC OF THE AQS ANIMAL EXPOSURE SYSTEM

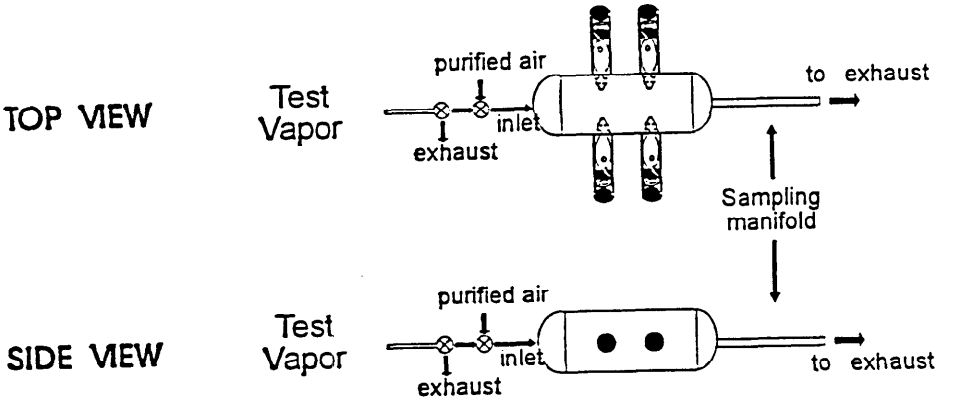


FIGURE 5

SIDE (A) AND TOP (B) VIEWS OF THE TEFLON® SEALING METHOD, AND METHOD FOR SECURING SOLID COLLAR TO GLASS TUBE (C)

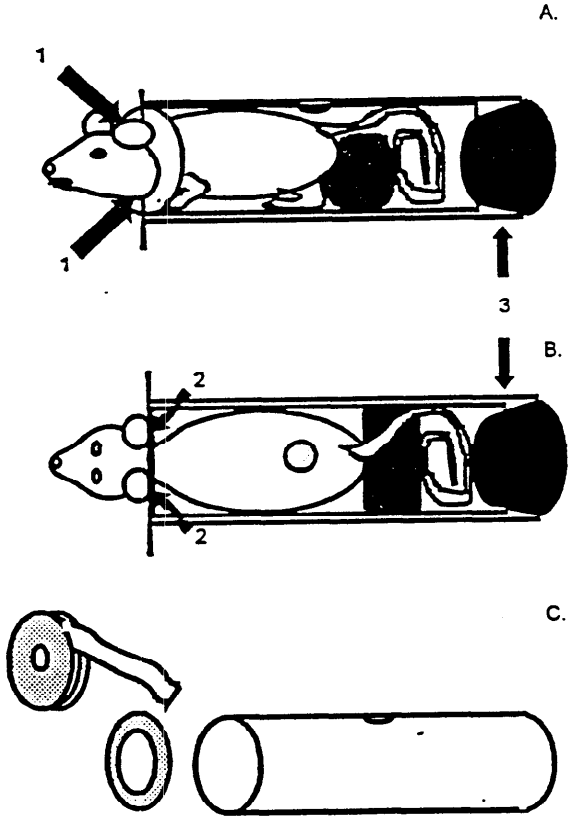
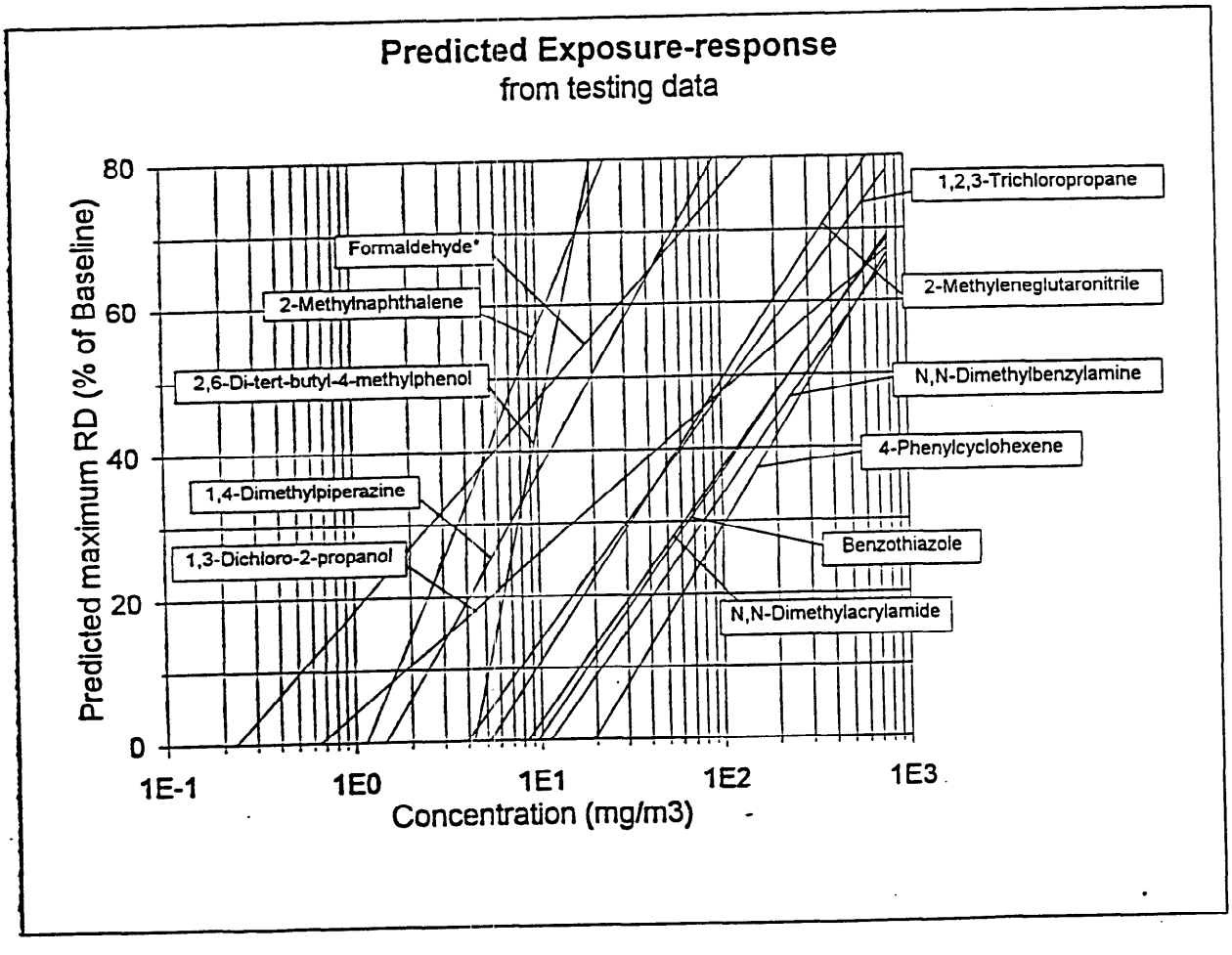


FIGURE 6



*Formaldehyde tested as positive control for sensory irritation; data presented to allow comparison of potency of Task 1 compounds with known irritant

FIGURE 7

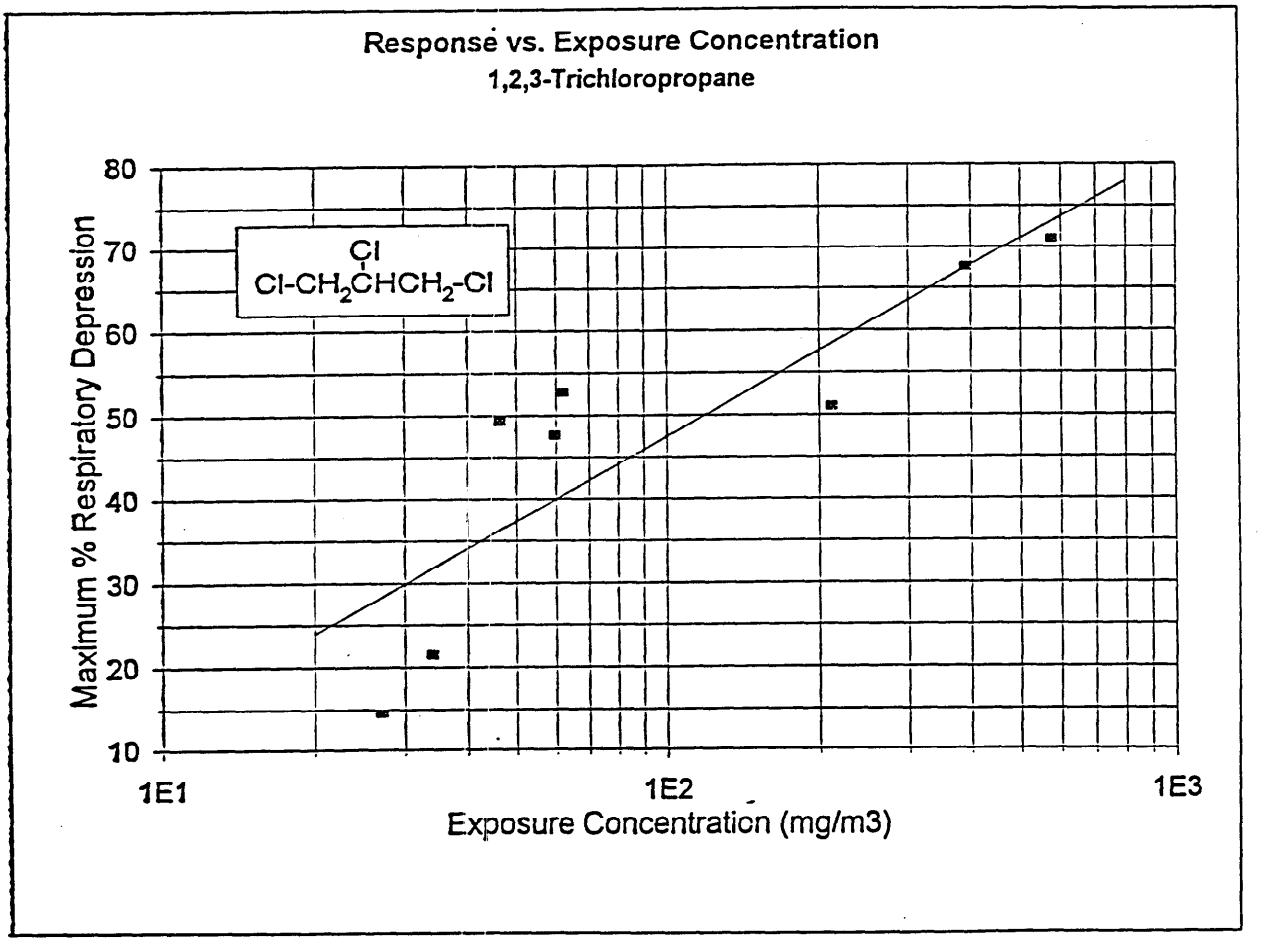

Response vs. Exposure Concentration
1,2,3-Trichloropropane
Cl
Cl-CH2CHCH2-Cl
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
1E1
1E2
1E3
Exposure Concentration (mg/m3)

FIGURE 8

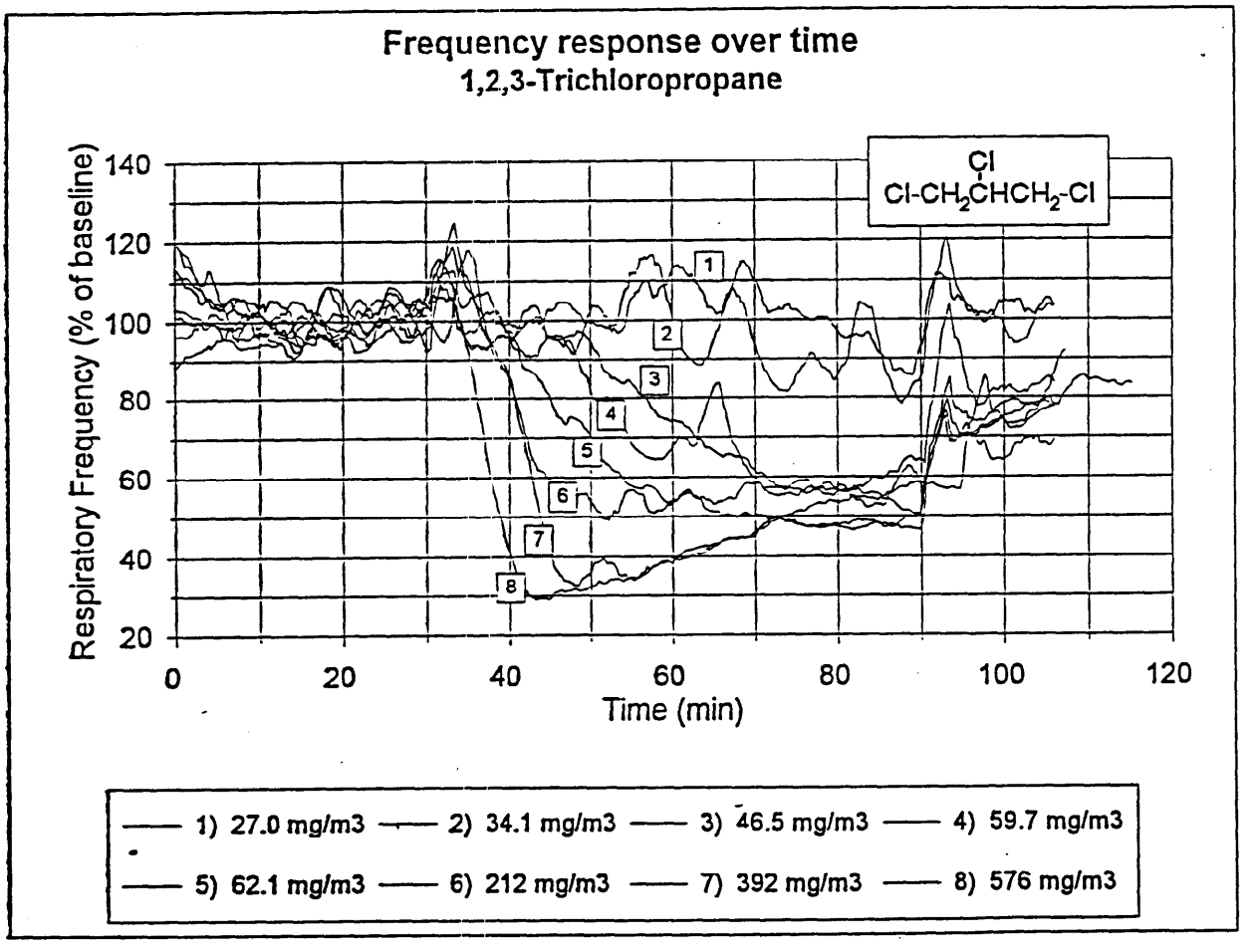

Frequency response over time
1,2,3-Trichloropropane
Cl
Cl-CH2CHCH2-Cl
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
6
7
8
1) 27.0 mg/m3
2) 34.1 mg/m3
3) 46.5 mg/m3
4) 59.7 mg/m3
5) 62.1 mg/m3
6) 212 mg/m3
7) 392 mg/m3
8) 576 mg/m3

FIGURE 9

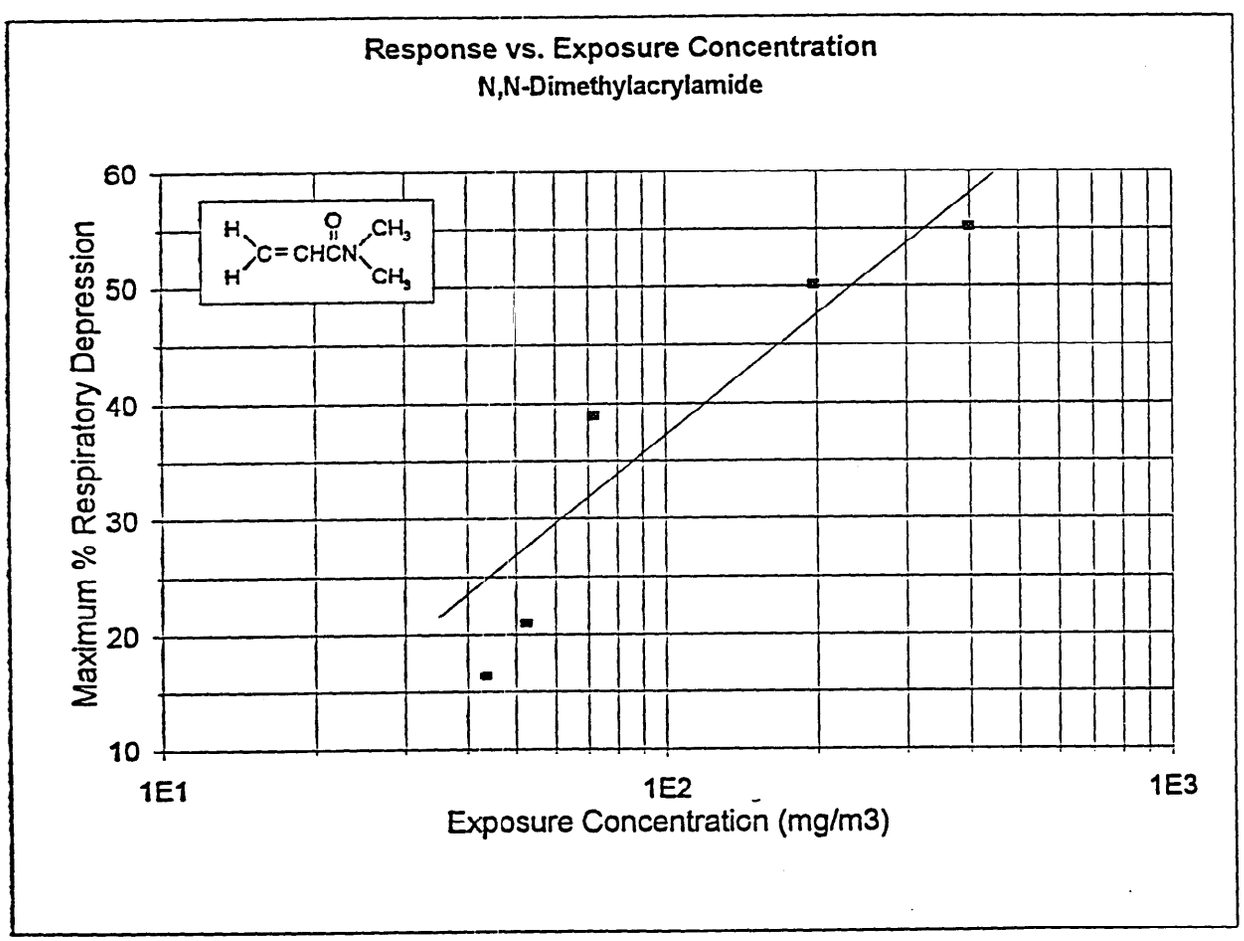

Response vs. Exposure Concentration
N,N-Dimethylacrylamide
Maximum % Respiratory Depression
60
50
40
30
20
10
1E1
1E2
1E3
Exposure Concentration (mg/m3)
H
H
C= CHCN
O
CH3
CH3

FIGURE 10

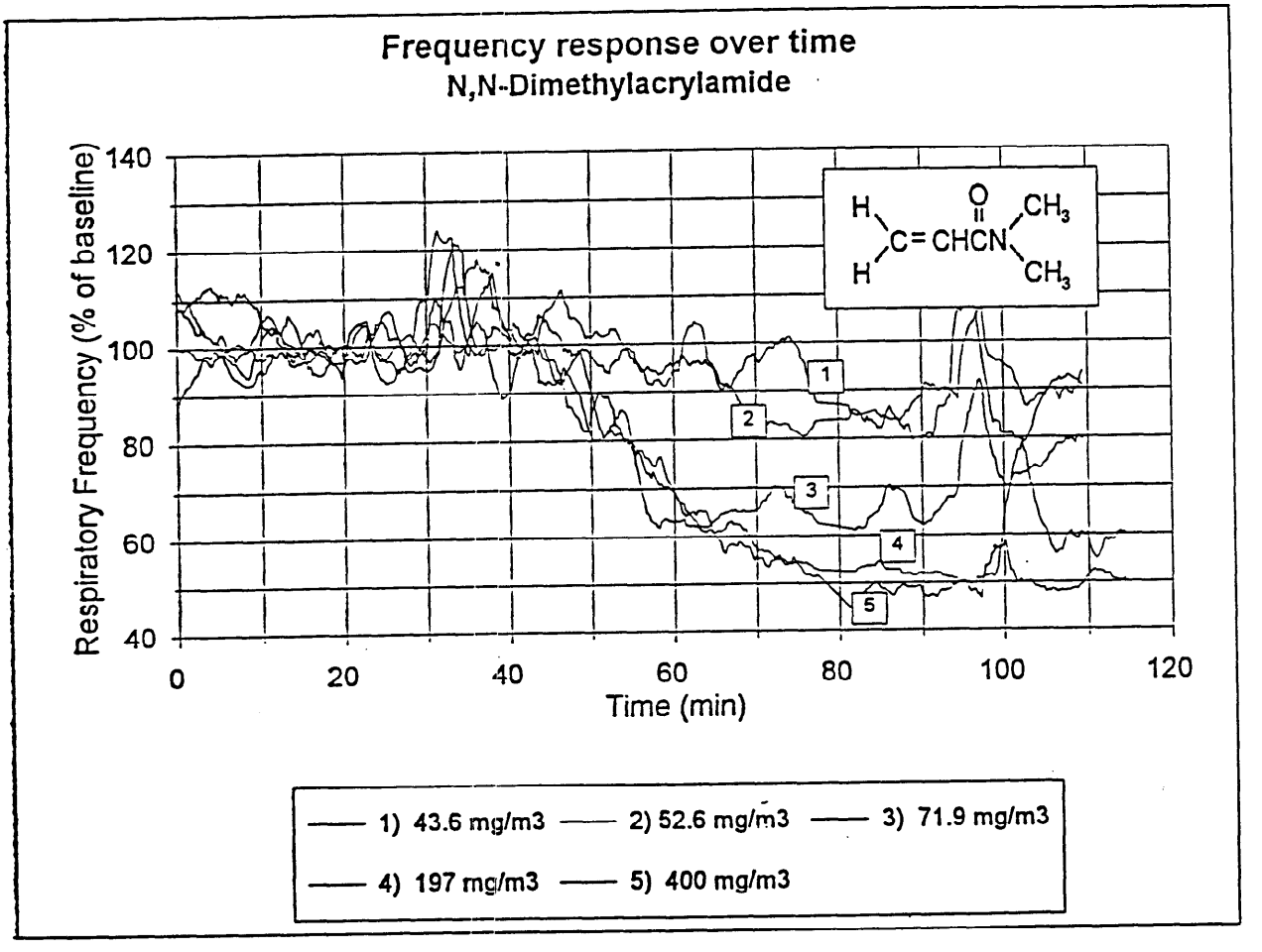

Frequency response over time
N,N-Dimethylacrylamide
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
1) 43.6 mg/m3
2) 52.6 mg/m3
3) 71.9 mg/m3
4) 197 mg/m3
5) 400 mg/m3

FIGURE 11

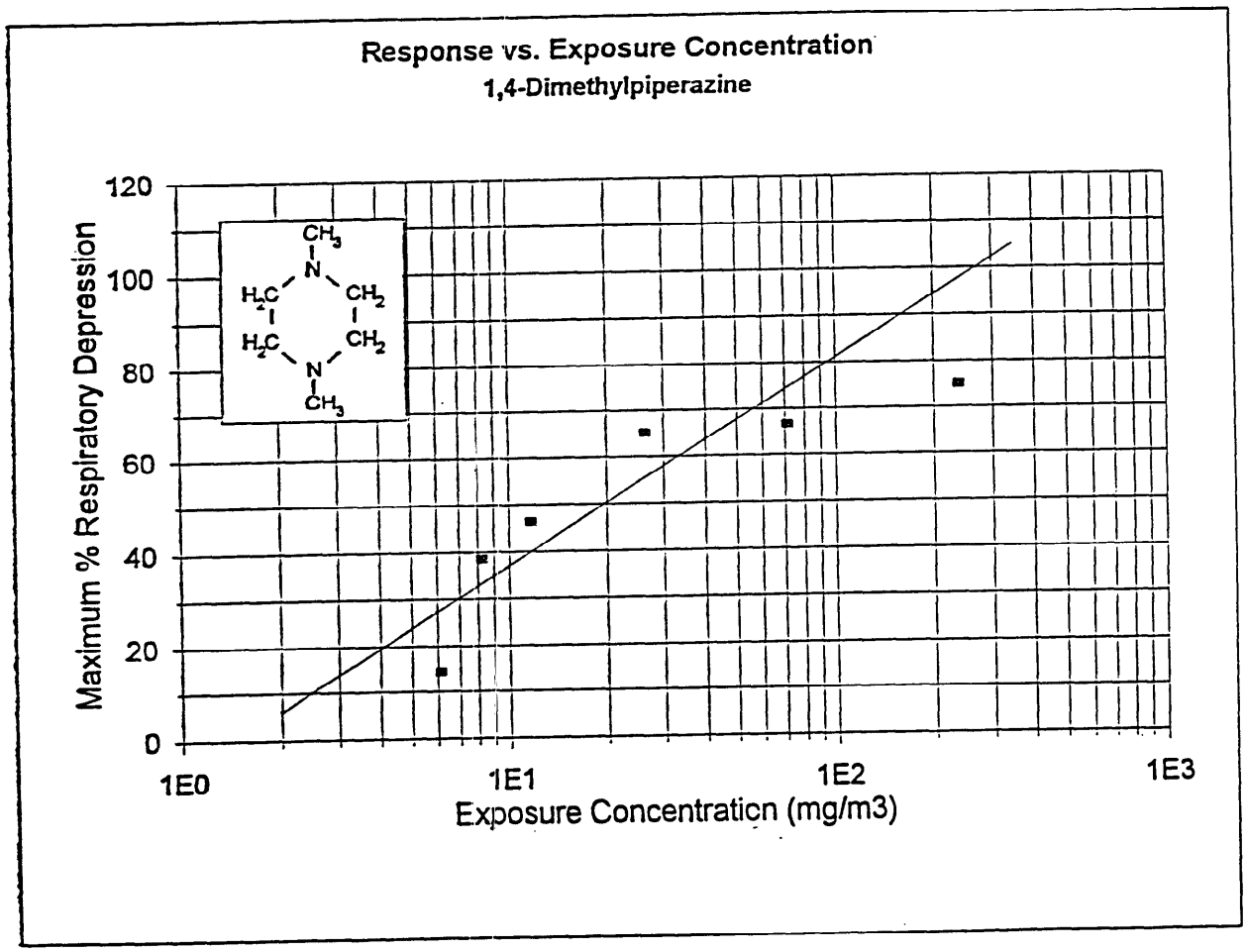

Response vs. Exposure Concentration
1,4-Dimethylpiperazine
Maximum % Respiratory Depression
120
100
80
60
40
20
0
1E0
1E1
1E2
1E3
Exposure Concentration (mg/m3)
CH3
N
H2C
CH2
H2C
CH2
N
CH3

FIGURE 12

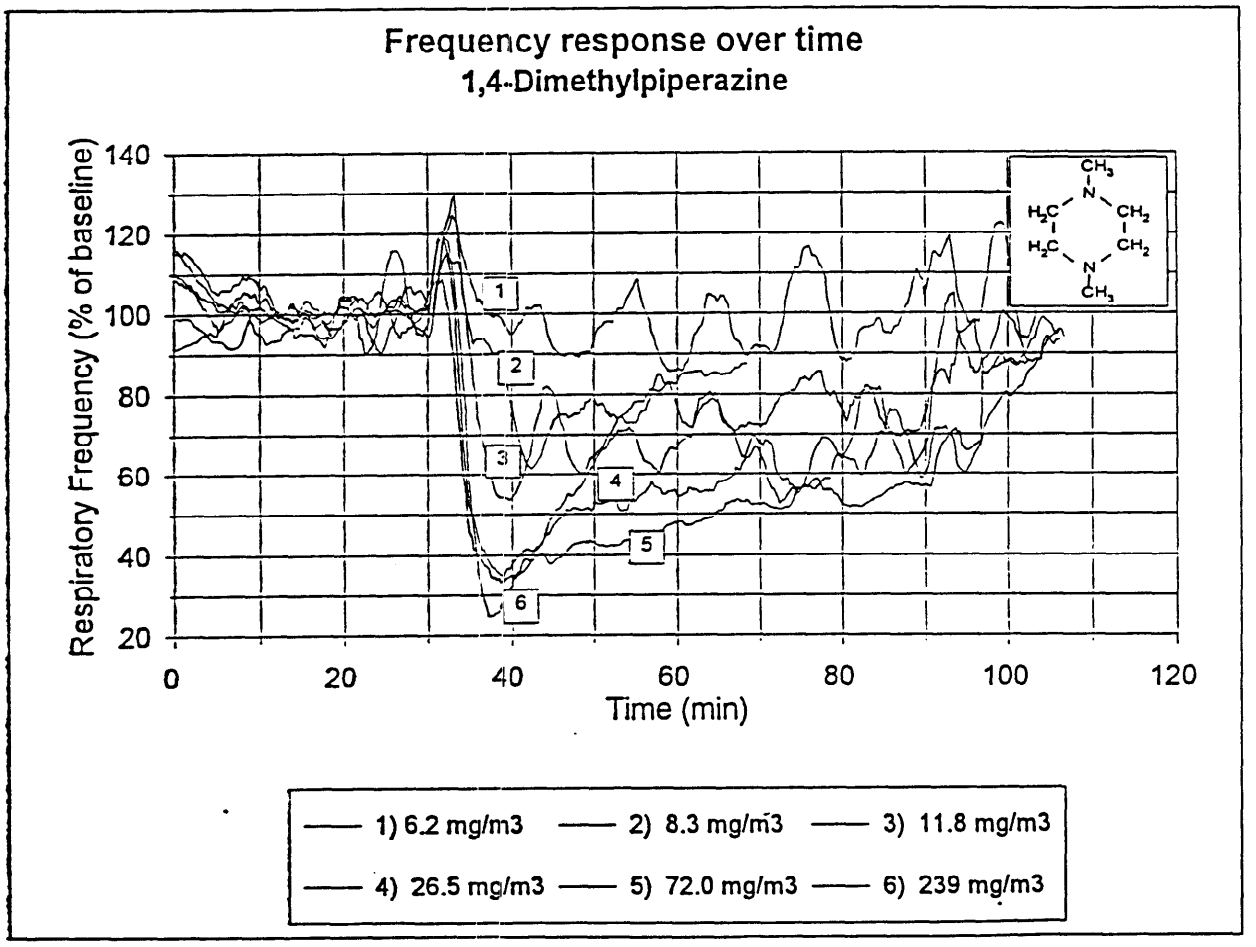

Frequency response over time
1,4-Dimethylpiperazine
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
6
1) 6.2 mg/m3
2) 8.3 mg/m3
3) 11.8 mg/m3
4) 26.5 mg/m3
5) 72.0 mg/m3
6) 239 mg/m3

FIGURE 13

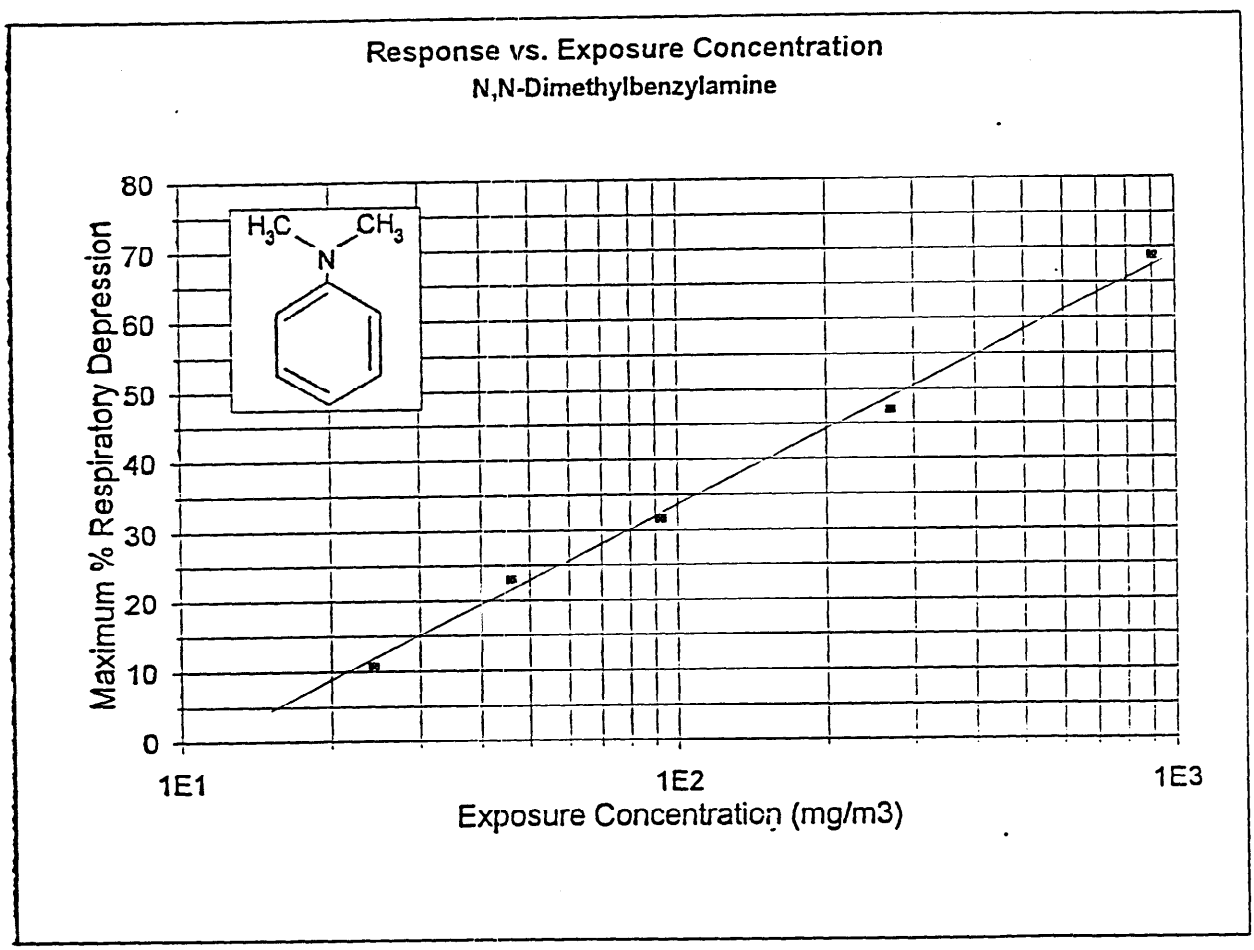

Response vs. Exposure Concentration
N,N-Dimethylbenzylamine
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
0
1E1
1E2
1E3
Exposure Concentration (mg/m3)
H3C
CH3
N

FIGURE 14

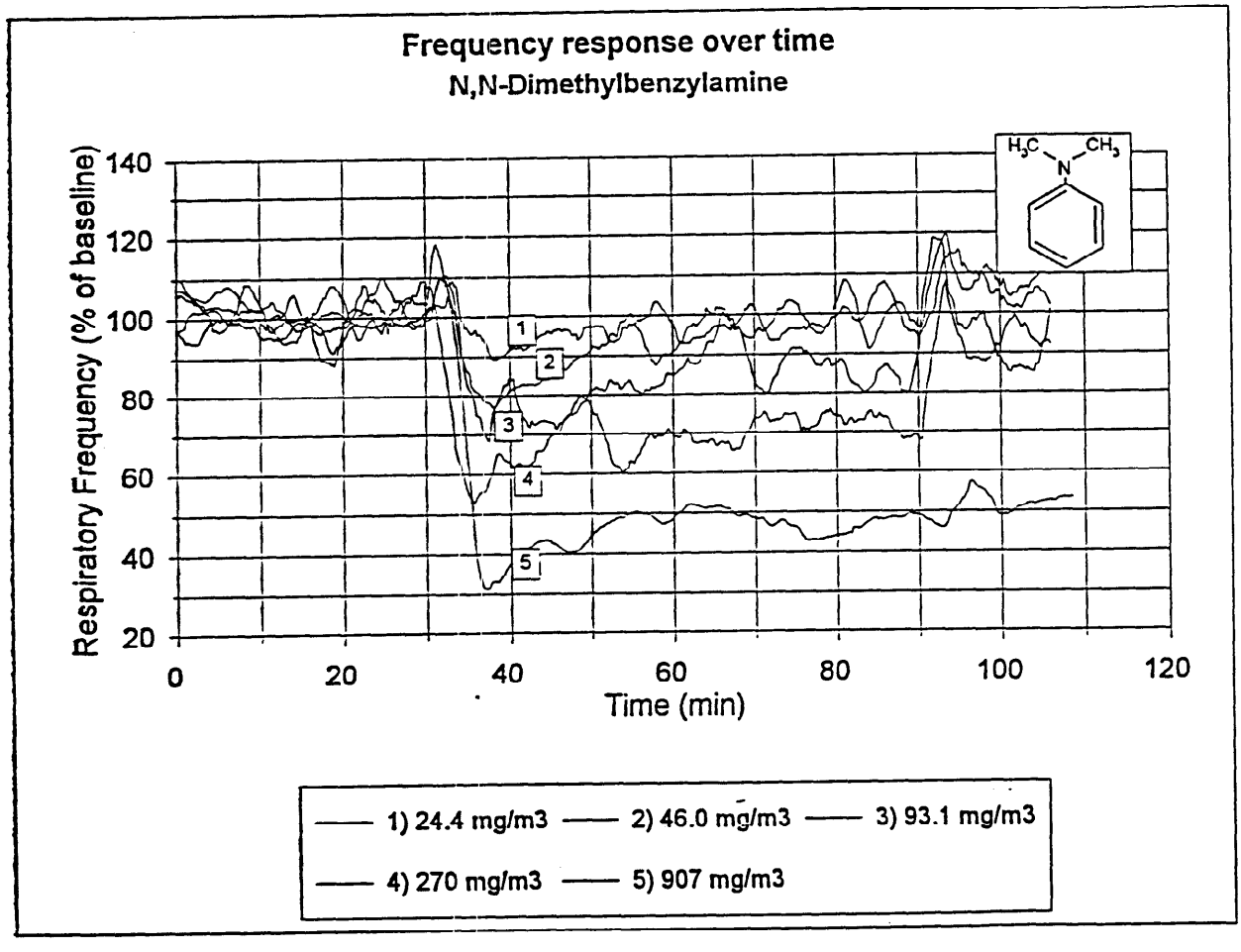

Frequency response over time
N,N-Dimethylbenzylamine
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
H3C
CH3
N
1) 24.4 mg/m3
2) 46.0 mg/m3
3) 93.1 mg/m3
4) 270 mg/m3
5) 907 mg/m3

FIGURE 15

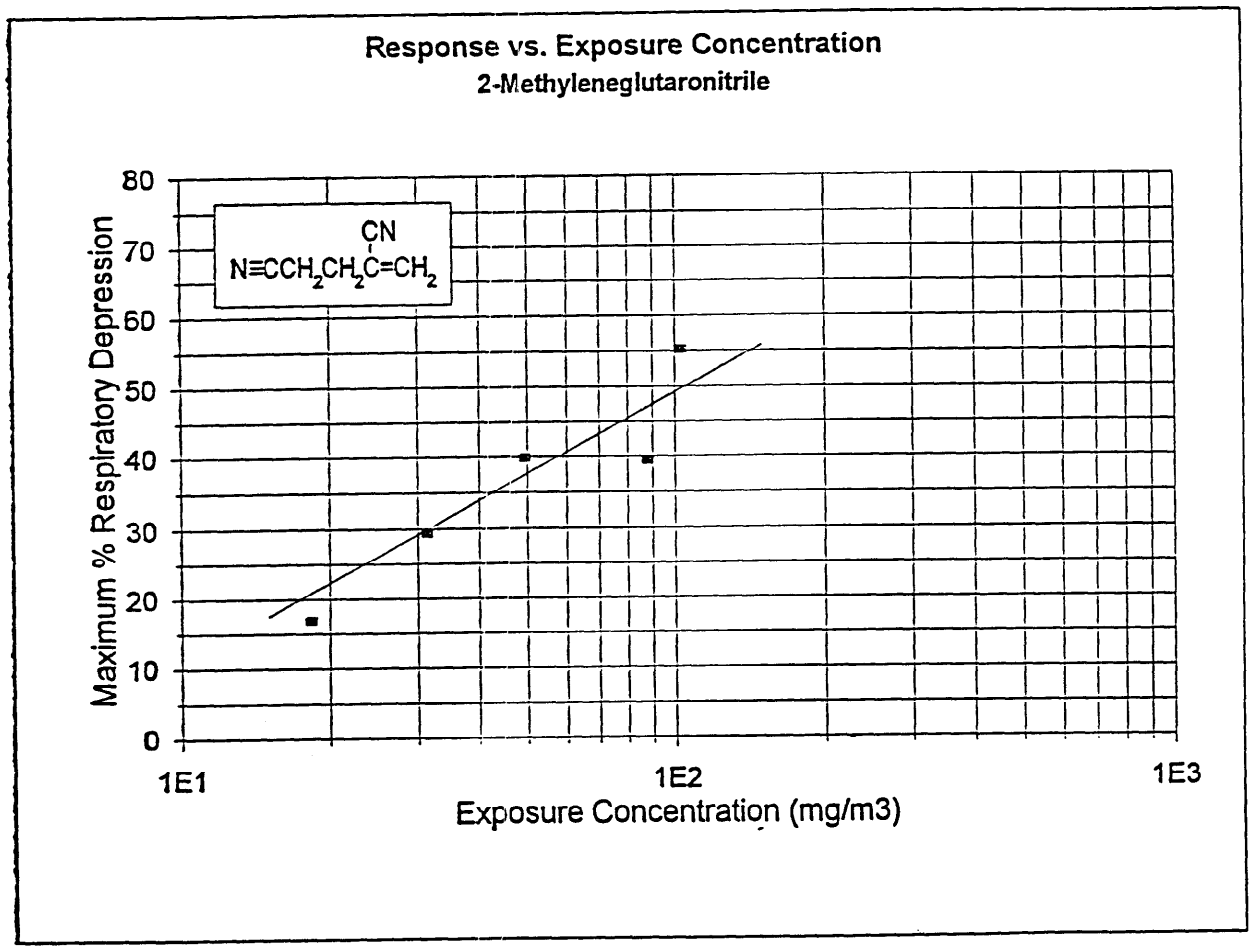

Response vs. Exposure Concentration
2-Methyleneglutaronitrile
CN
N≡CCH2CH2C=CH2
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
0
1E1
1E2
1E3
Exposure Concentration (mg/m3)

FIGURE 16

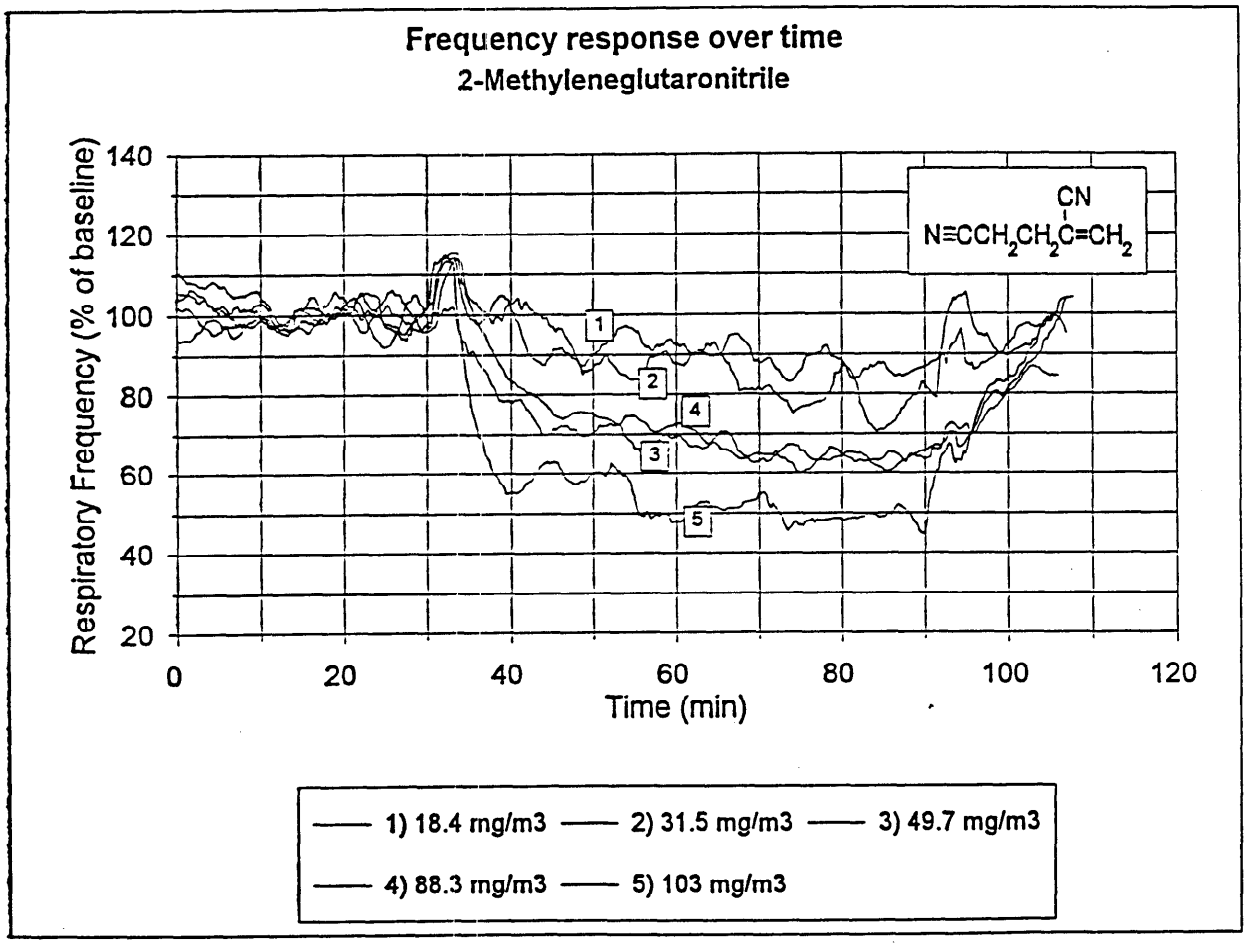

Frequency response over time
2-Methyleneglutaronitrile
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
CN
N≡CCH2CH2C=CH2
1
2
3
4
5
1) 18.4 mg/m3
2) 31.5 mg/m3
3) 49.7 mg/m3
4) 88.3 mg/m3
5) 103 mg/m3

FIGURE 17

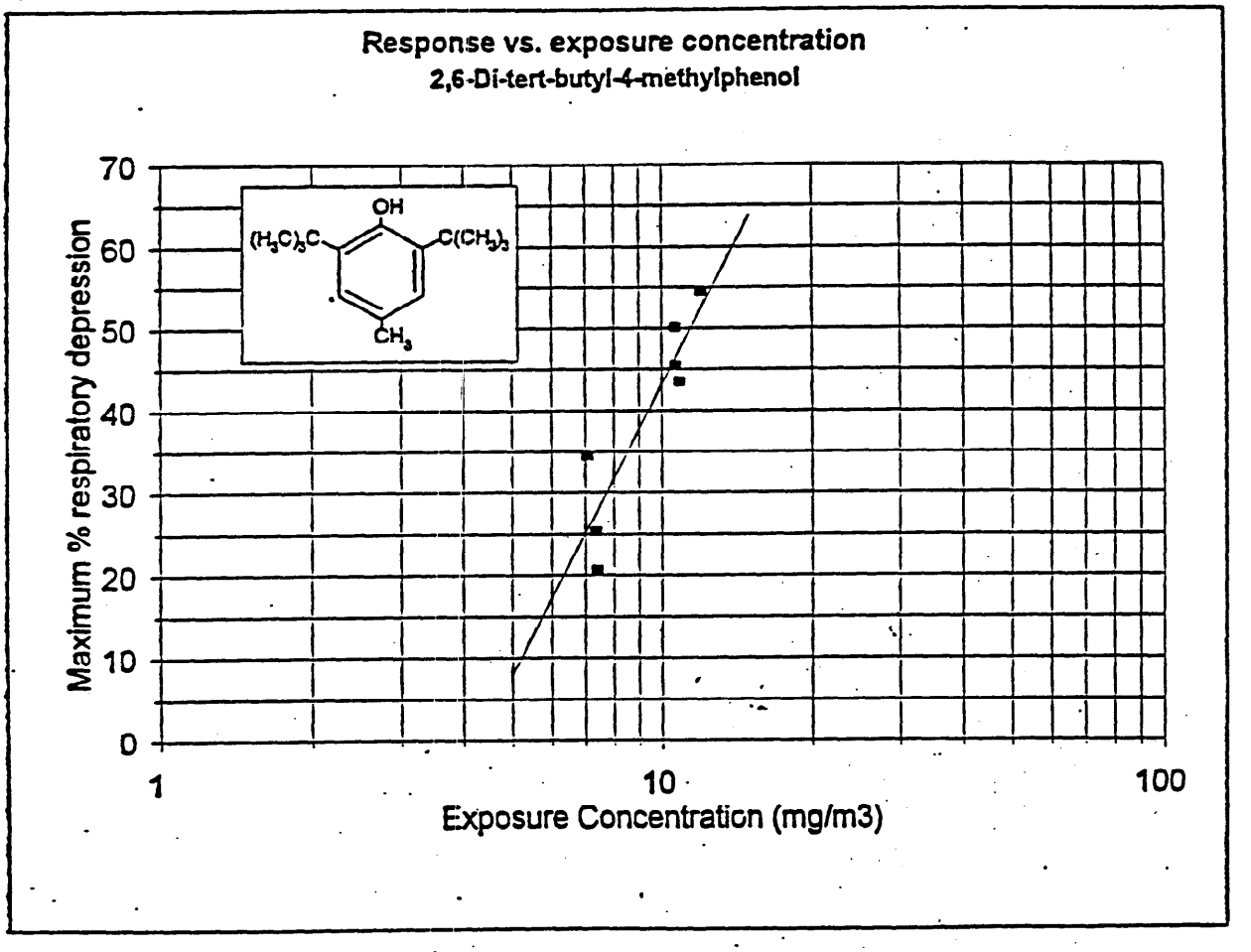

Response vs. exposure concentration
2,6-Di-tert-butyl-4-methylphenol
Maximum % respiratory depression
70
60
50
40
30
20
10
0
1
10
100
Exposure Concentration (mg/m3)
OH
(H3C)3C
C(CH3)3
CH3

FIGURE 18

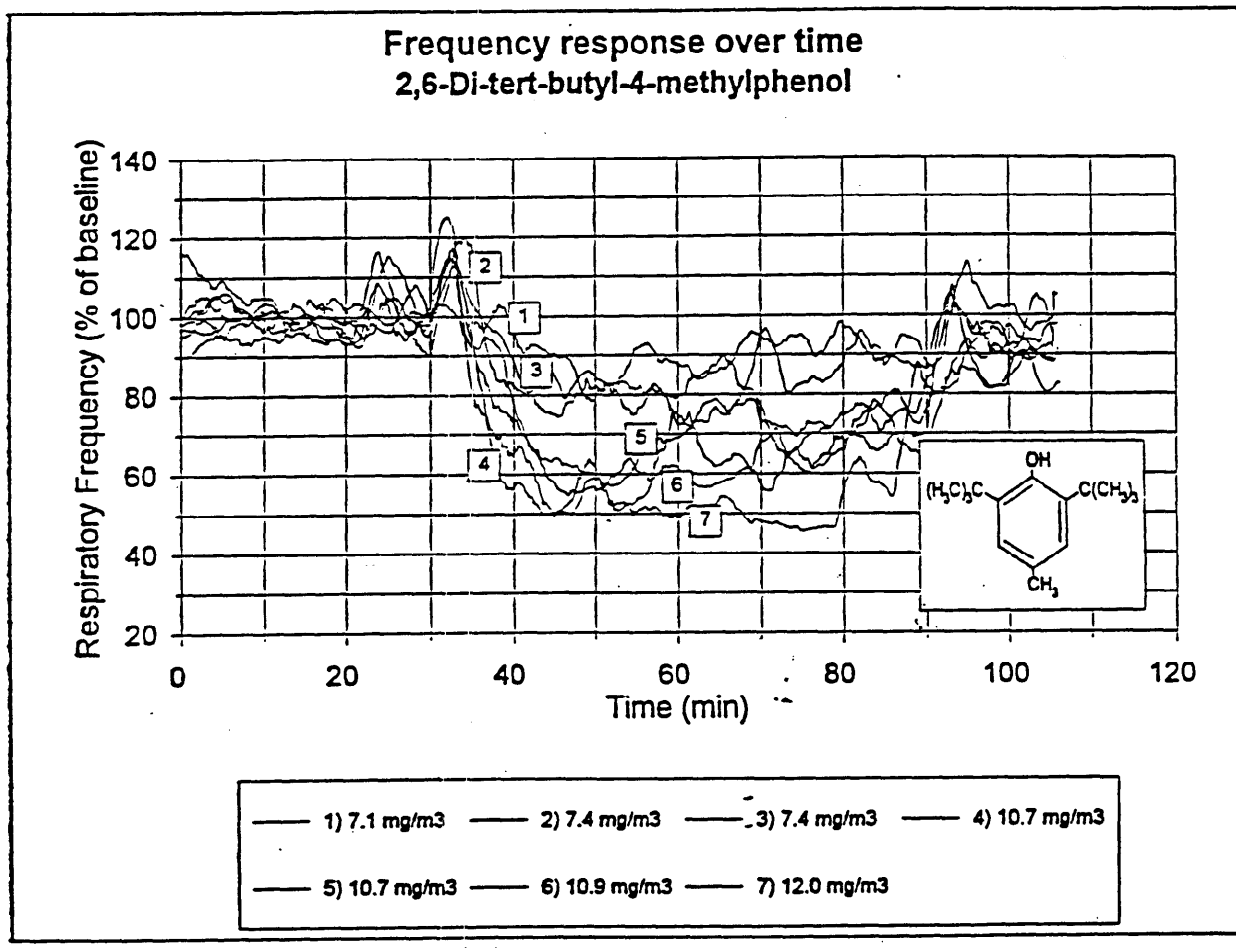

Frequency response over time
2,6-Di-tert-butyl-4-methylphenol
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
6
7
OH
(H3C)3C
C(CH3)3
CH3
1) 7.1 mg/m3
2) 7.4 mg/m3
3) 7.4 mg/m3
4) 10.7 mg/m3
5) 10.7 mg/m3
6) 10.9 mg/m3
7) 12.0 mg/m3

FIGURE 19

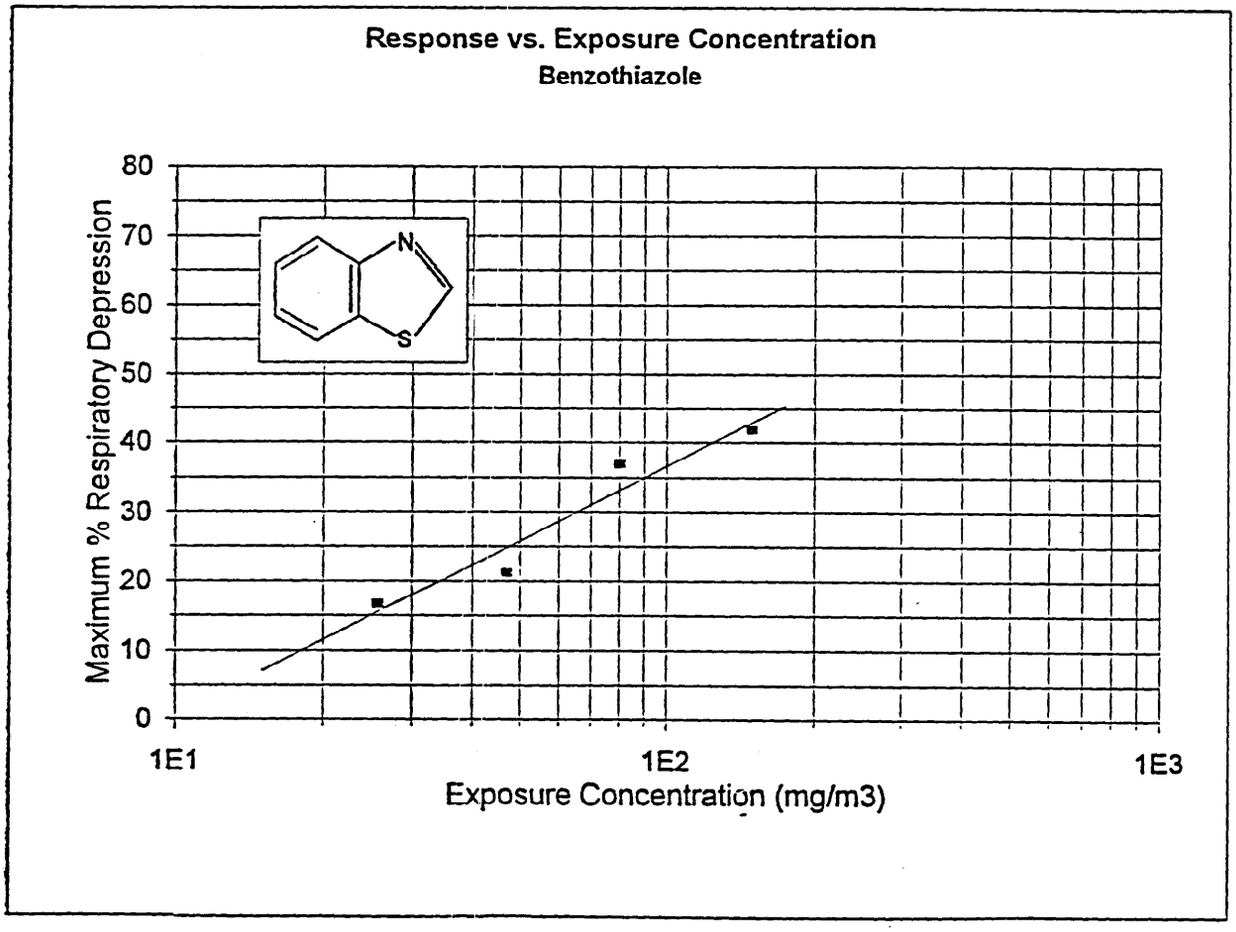

Response vs. Exposure Concentration
Benzothiazole
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
0
N
S
1E1
1E2
1E3
Exposure Concentration (mg/m3)

FIGURE 20

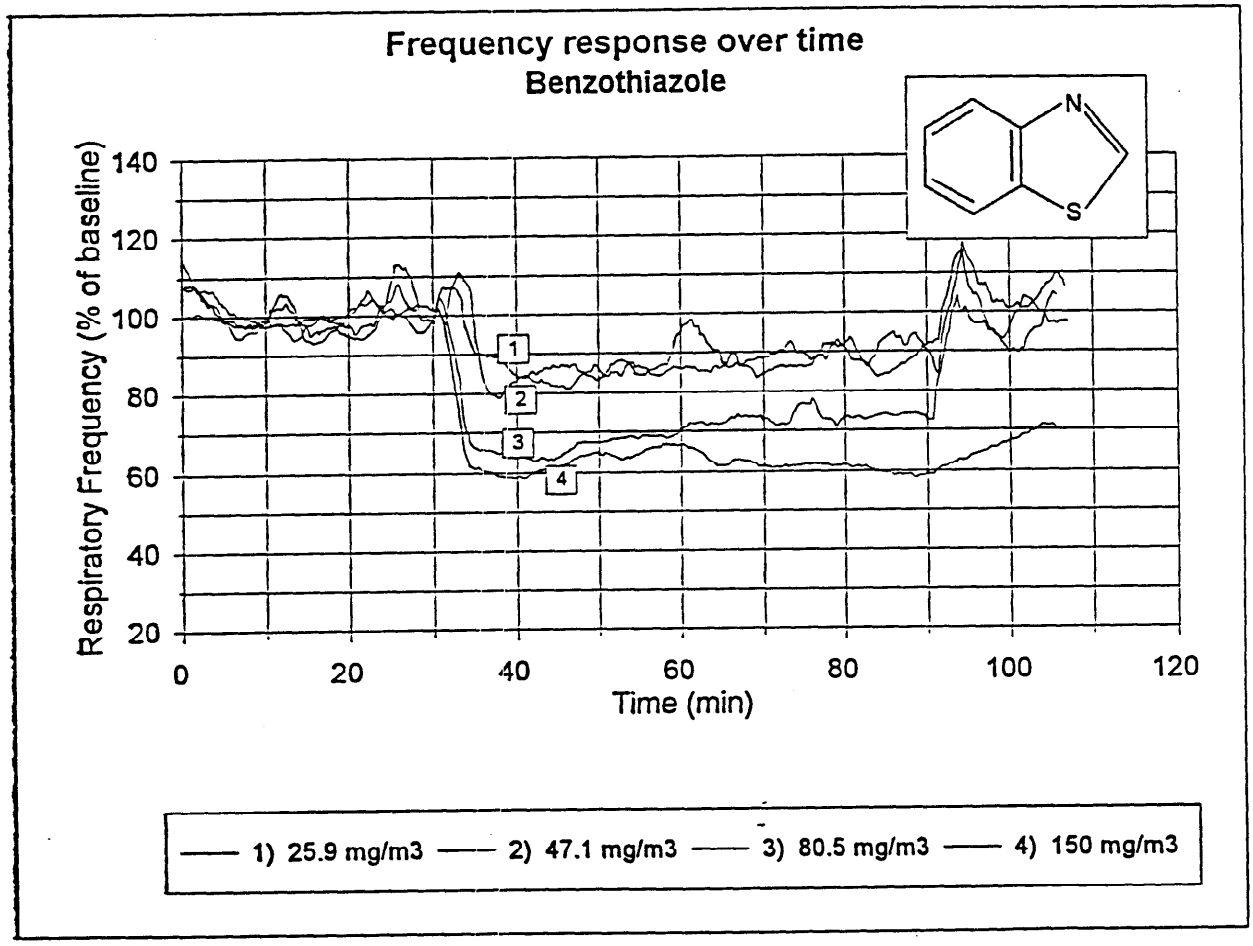

Frequency response over time
Benzothiazole
N
S
Respiratory Frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
1) 25.9 mg/m3
2) 47.1 mg/m3
3) 80.5 mg/m3
4) 150 mg/m3

FIGURE 21

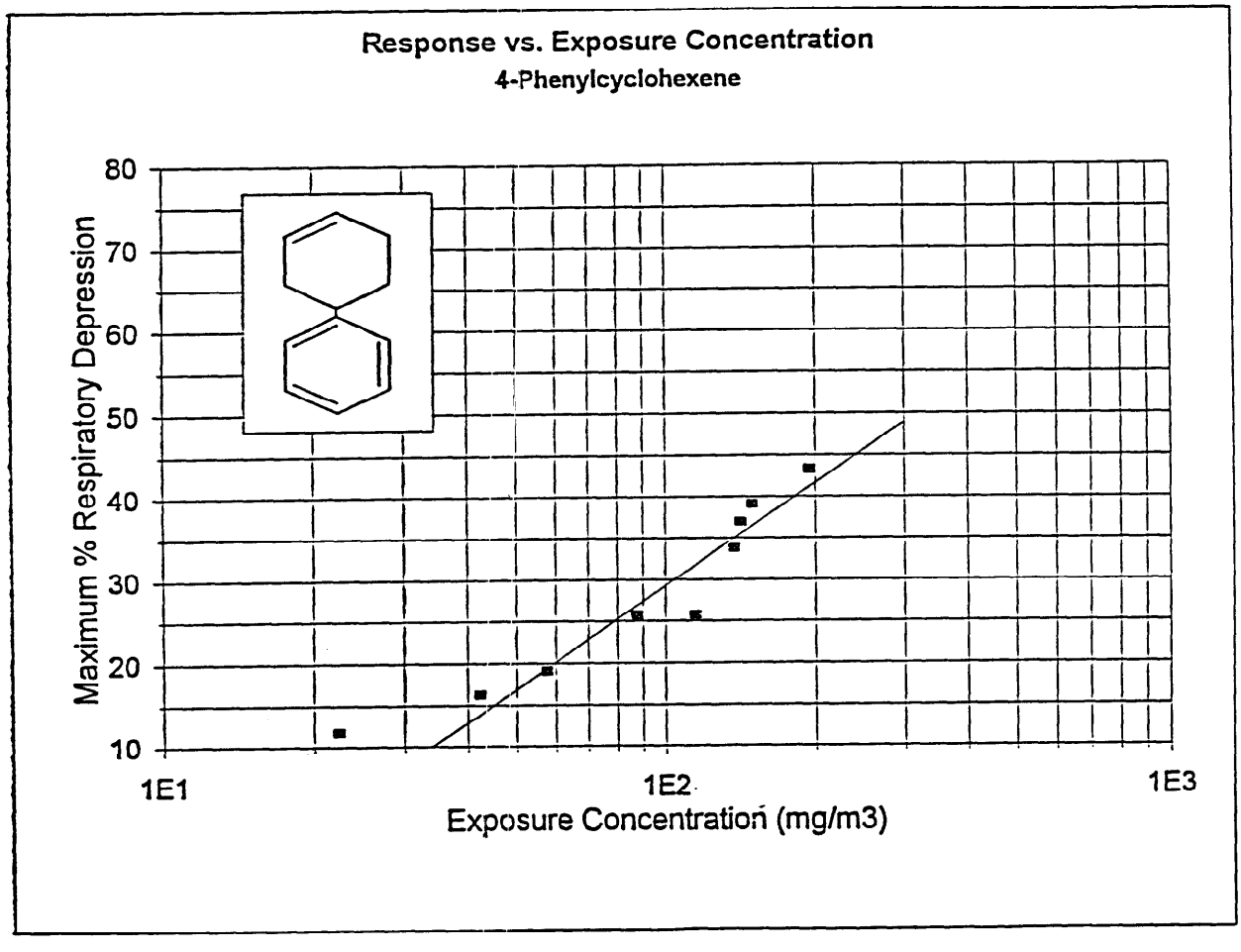

Response vs. Exposure Concentration
4-Phenylcyclohexene
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
1E1
1E2
1E3
Exposure Concentration (mg/m3)

FIGURE 22

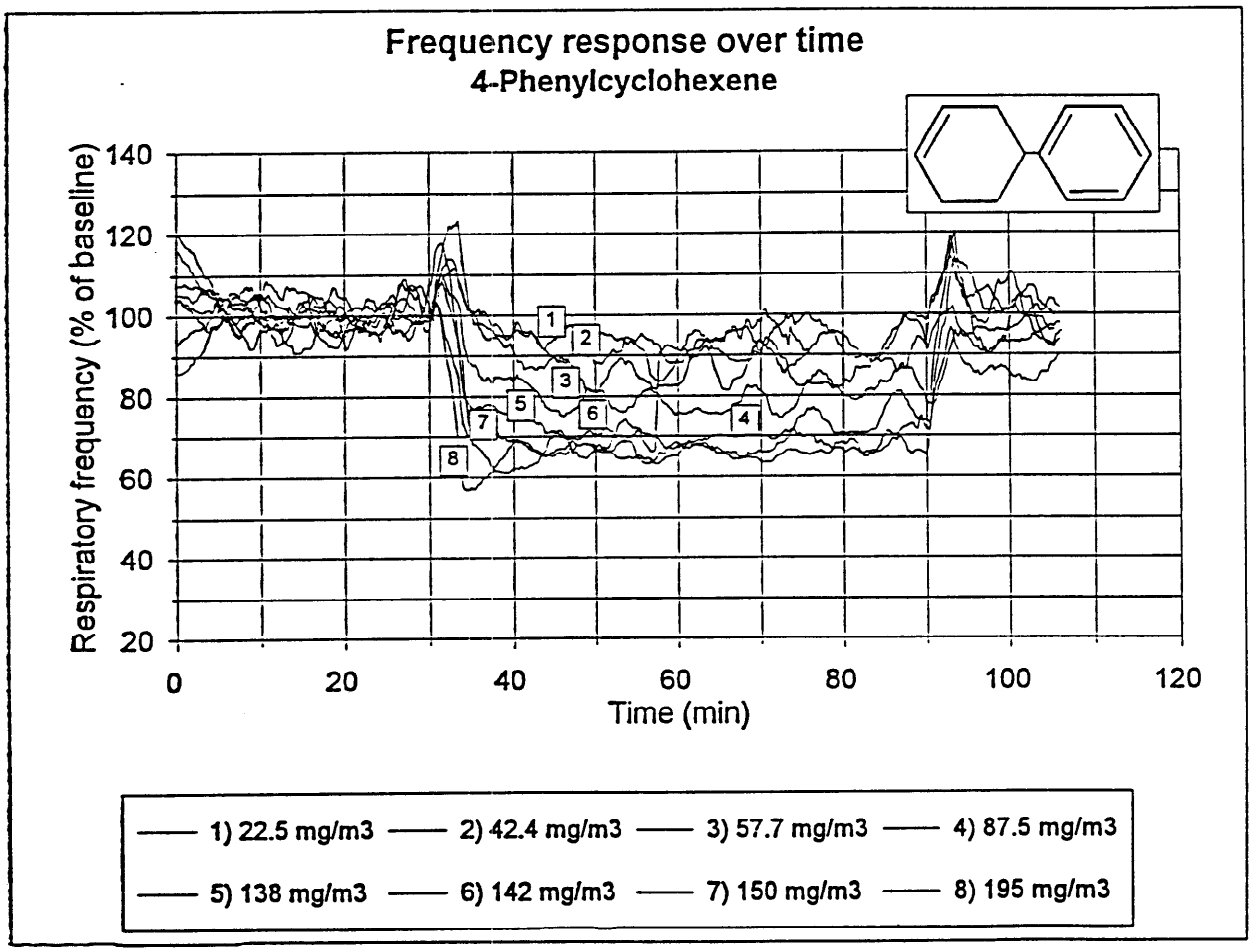

Frequency response over time
4-Phenylcyclohexene
Respiratory frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
6
7
8
1) 22.5 mg/m3
2) 42.4 mg/m3
3) 57.7 mg/m3
4) 87.5 mg/m3
5) 138 mg/m3
6) 142 mg/m3
7) 150 mg/m3
8) 195 mg/m3

FIGURE 23

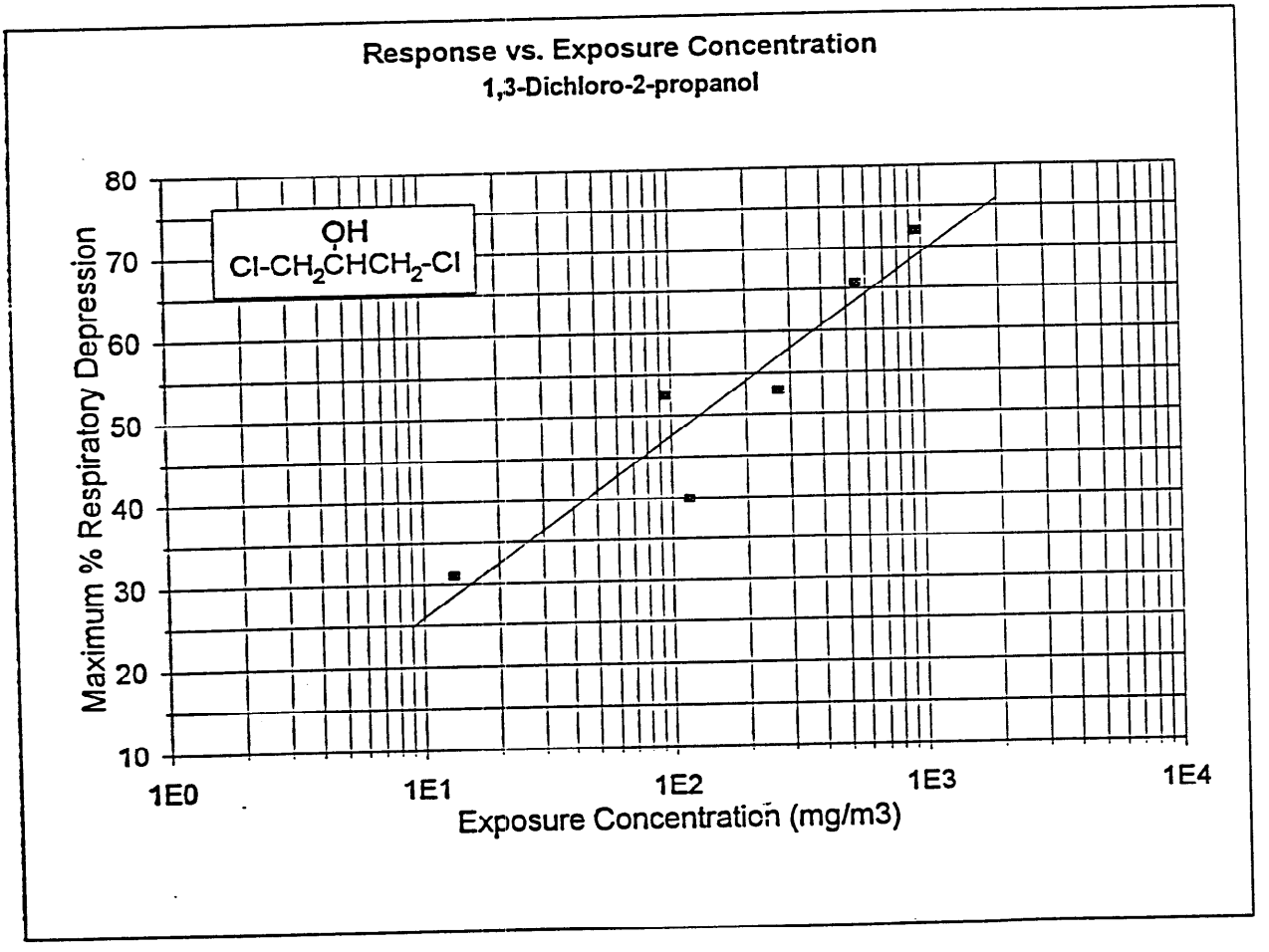

Response vs. Exposure Concentration
1,3-Dichloro-2-propanol
OH
Cl-CH2CHCH2-Cl
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
1E0
1E1
1E2
1E3
1E4
Exposure Concentration (mg/m3)

FIGURE 24

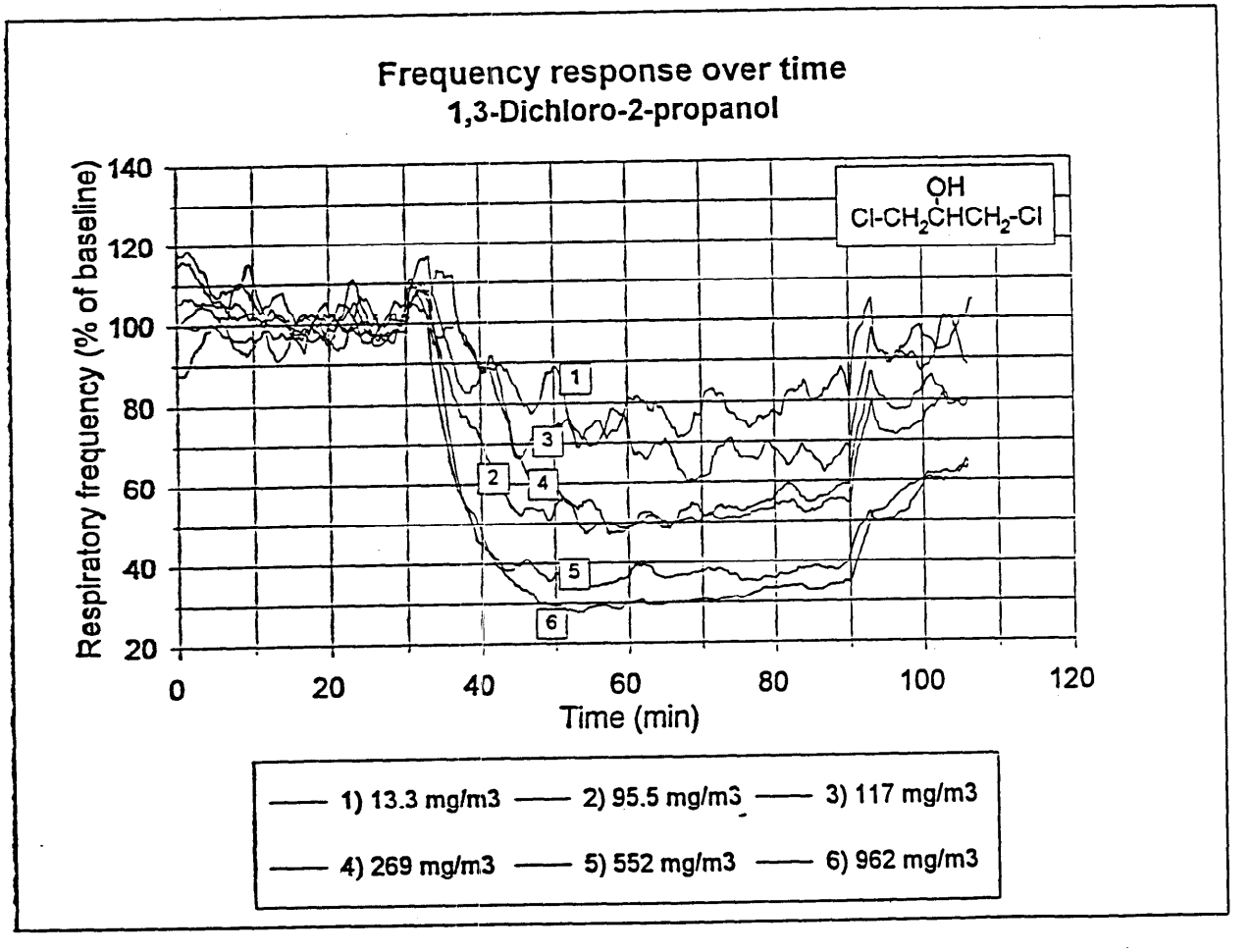

Frequency response over time
1,3-Dichloro-2-propanol
OH
Cl-CH2CHCH2-Cl
Respiratory frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
1
2
3
4
5
6
1) 13.3 mg/m3
2) 95.5 mg/m3
3) 117 mg/m3
4) 269 mg/m3
5) 552 mg/m3
6) 962 mg/m3

FIGURE 25

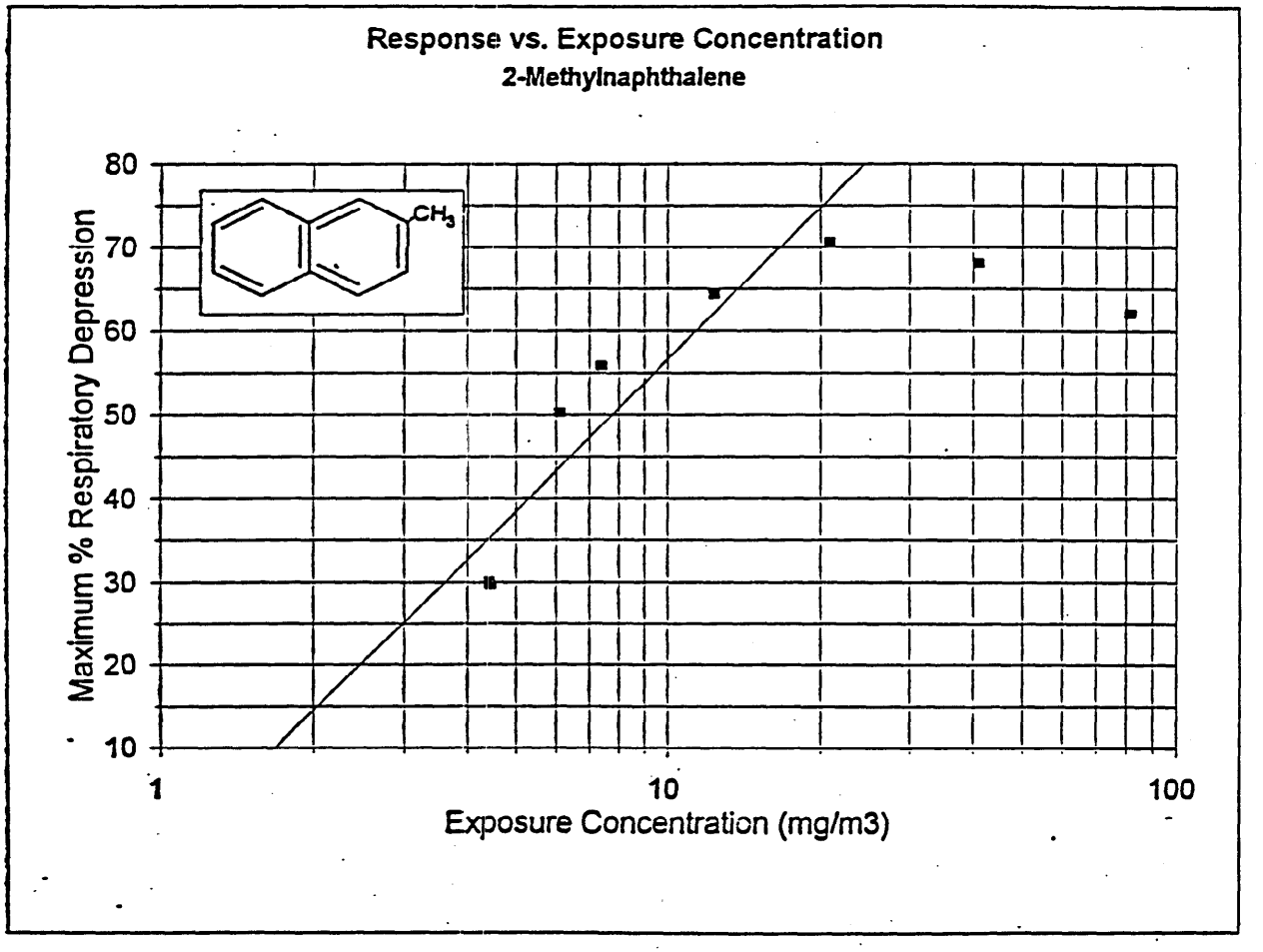

Response vs. Exposure Concentration
2-Methylnaphthalene
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
1
10
100
Exposure Concentration (mg/m3)
CH3

FIGURE 26

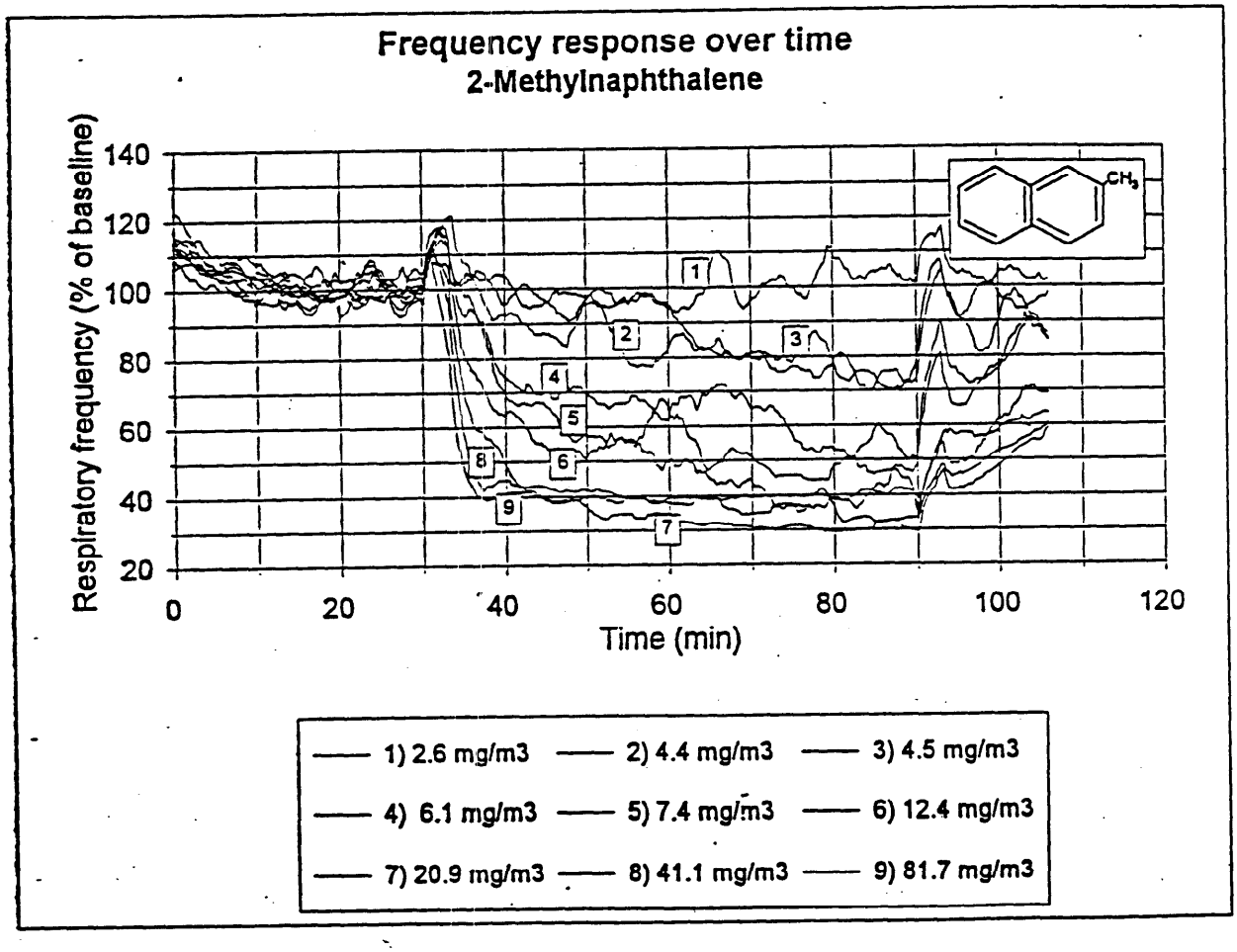

Frequency response over time
2-Methylnaphthalene
Respiratory frequency (% of baseline)
140
120
100
80
60
40
20
0
20
40
60
80
100
120
Time (min)
CH3
1
2
3
4
5
6
7
8
9
1) 2.6 mg/m3
2) 4.4 mg/m3
3) 4.5 mg/m3
4) 6.1 mg/m3
5) 7.4 mg/m3
6) 12.4 mg/m3
7) 20.9 mg/m3
8) 41.1 mg/m3
9) 81.7 mg/m3

FIGURE 27

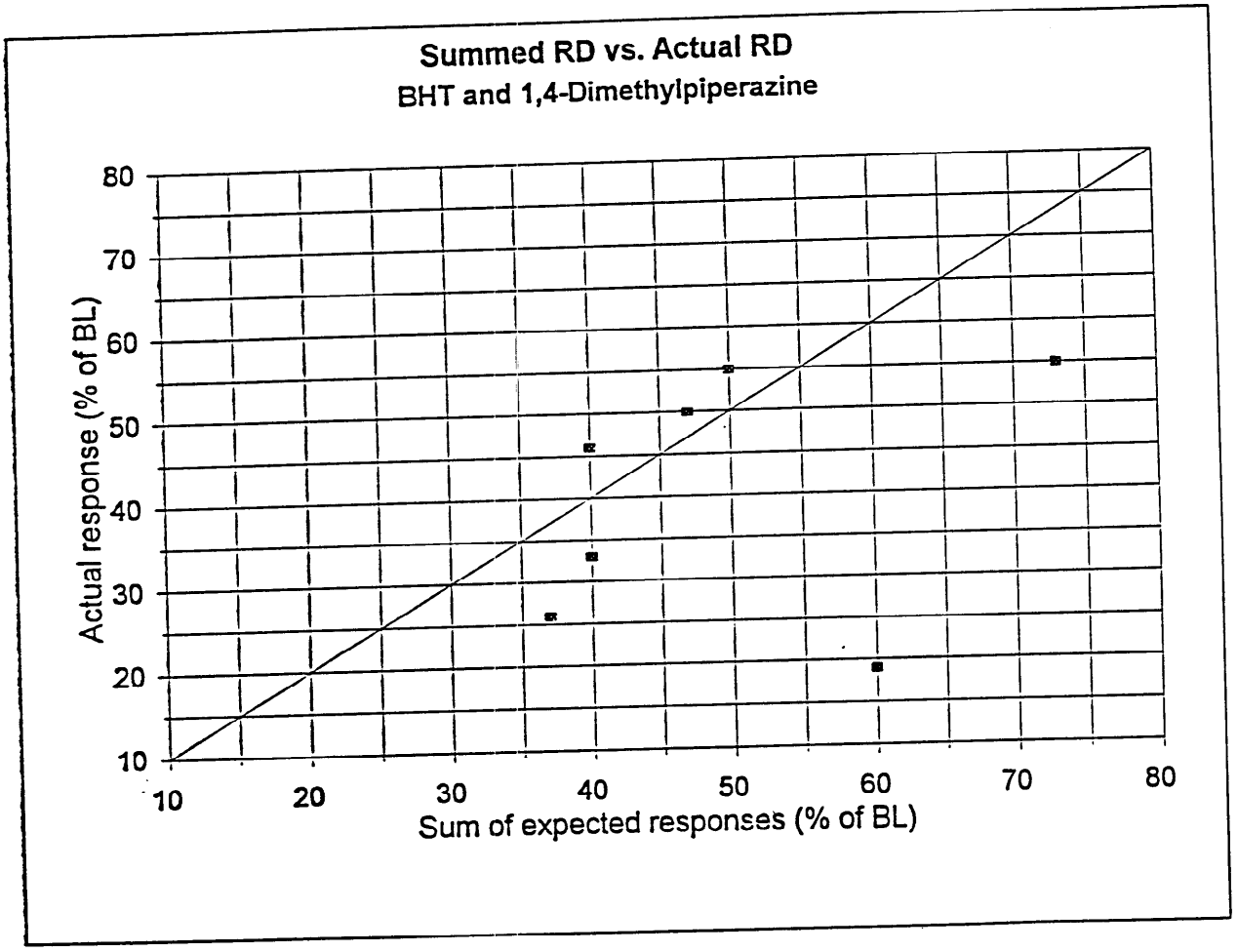

Summed RD vs. Actual RD
BHT and 1,4-Dimethylpiperazine
Actual response (% of BL)
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
Sum of expected responses (% of BL)

FIGURE 28

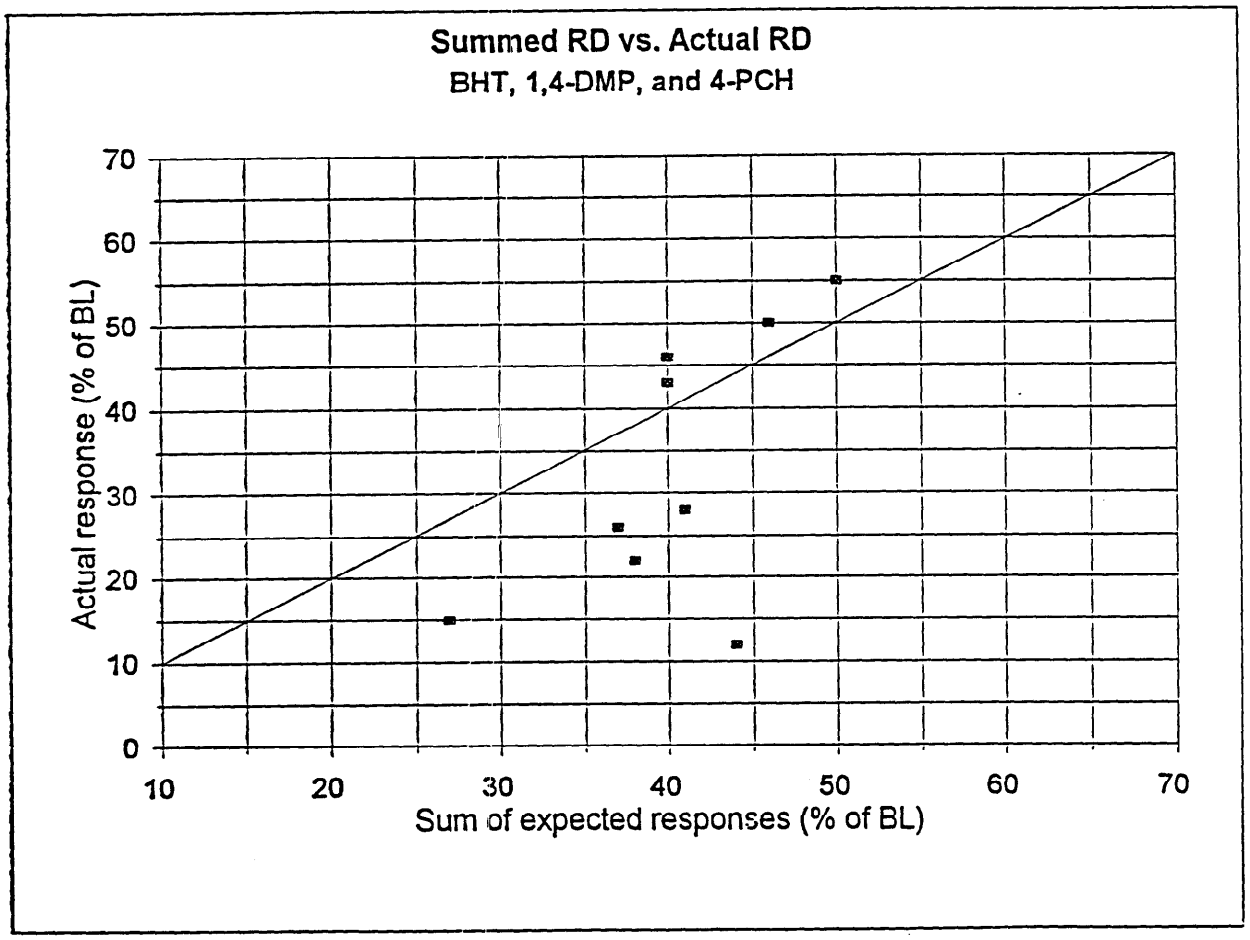

Summed RD vs. Actual RD
BHT, 1,4-DMP, and 4-PCH
Actual response (% of BL)
0
10
20
30
40
50
60
70
10
20
30
40
50
60
70
Sum of expected responses (% of BL)

FIGURE 29

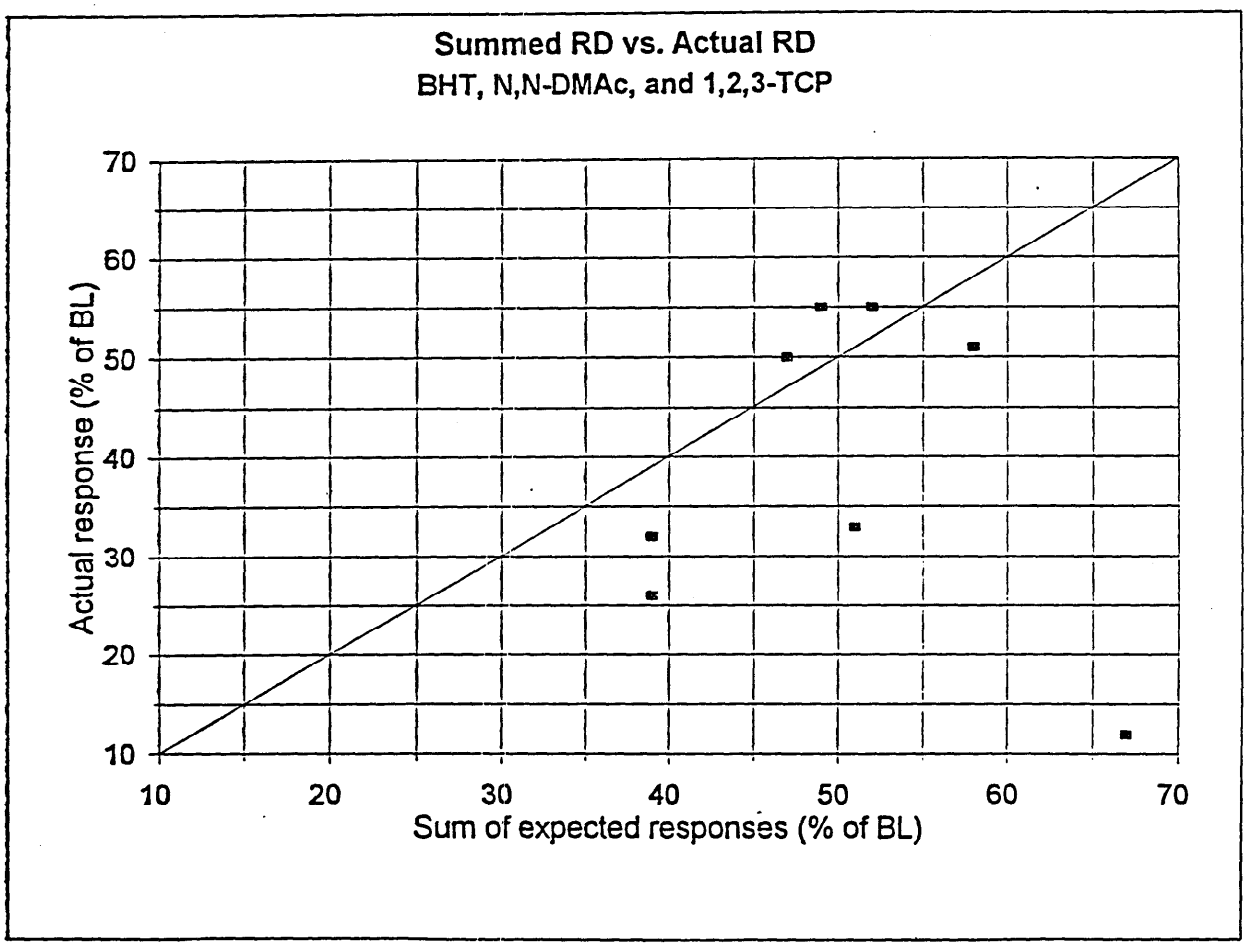

Summed RD vs. Actual RD
BHT, N,N-DMAc, and 1,2,3-TCP
Actual response (% of BL)
70
60
50
40
30
20
10
10
20
30
40
50
60
70
Sum of expected responses (% of BL)

FIGURE 30

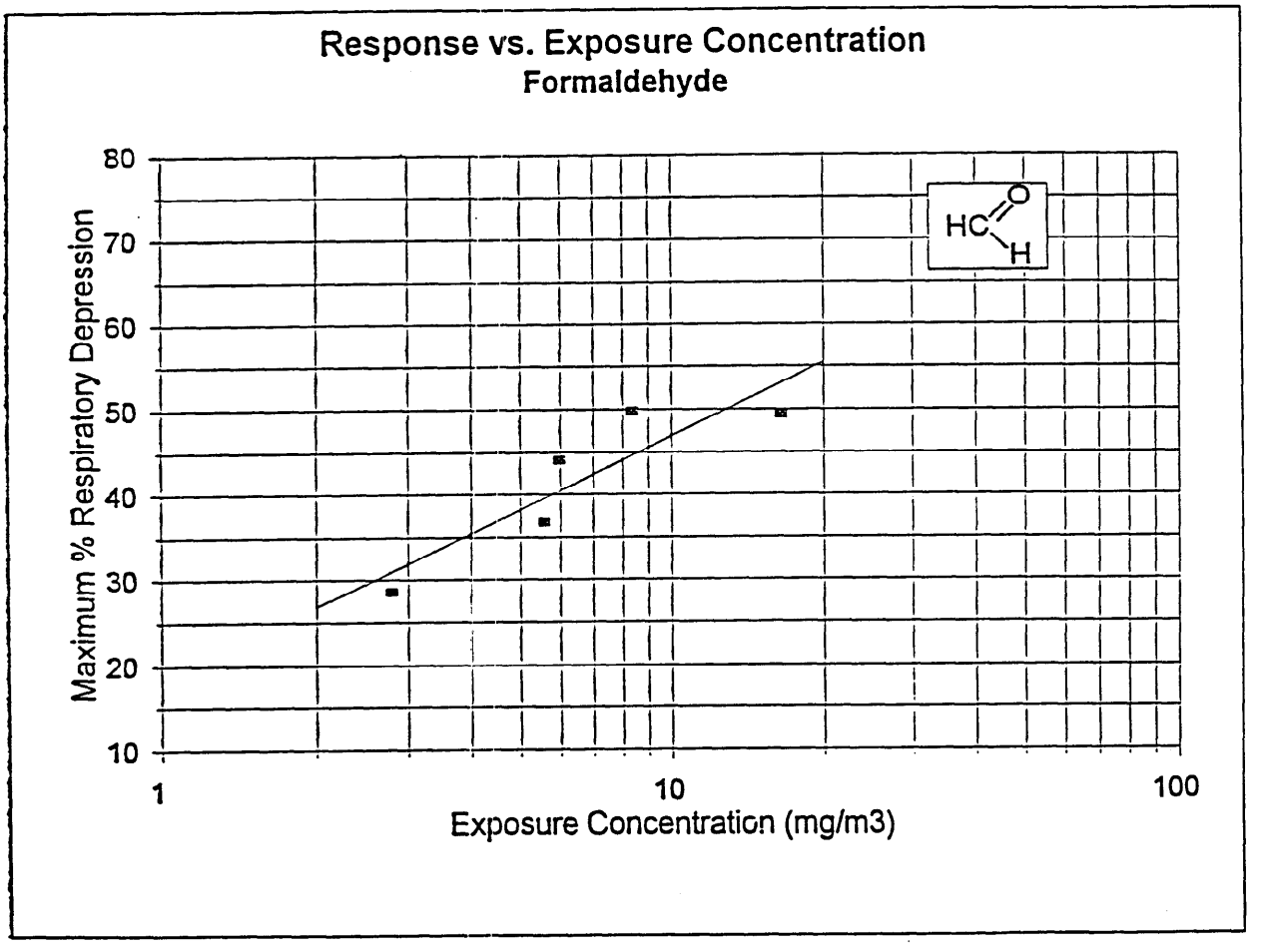
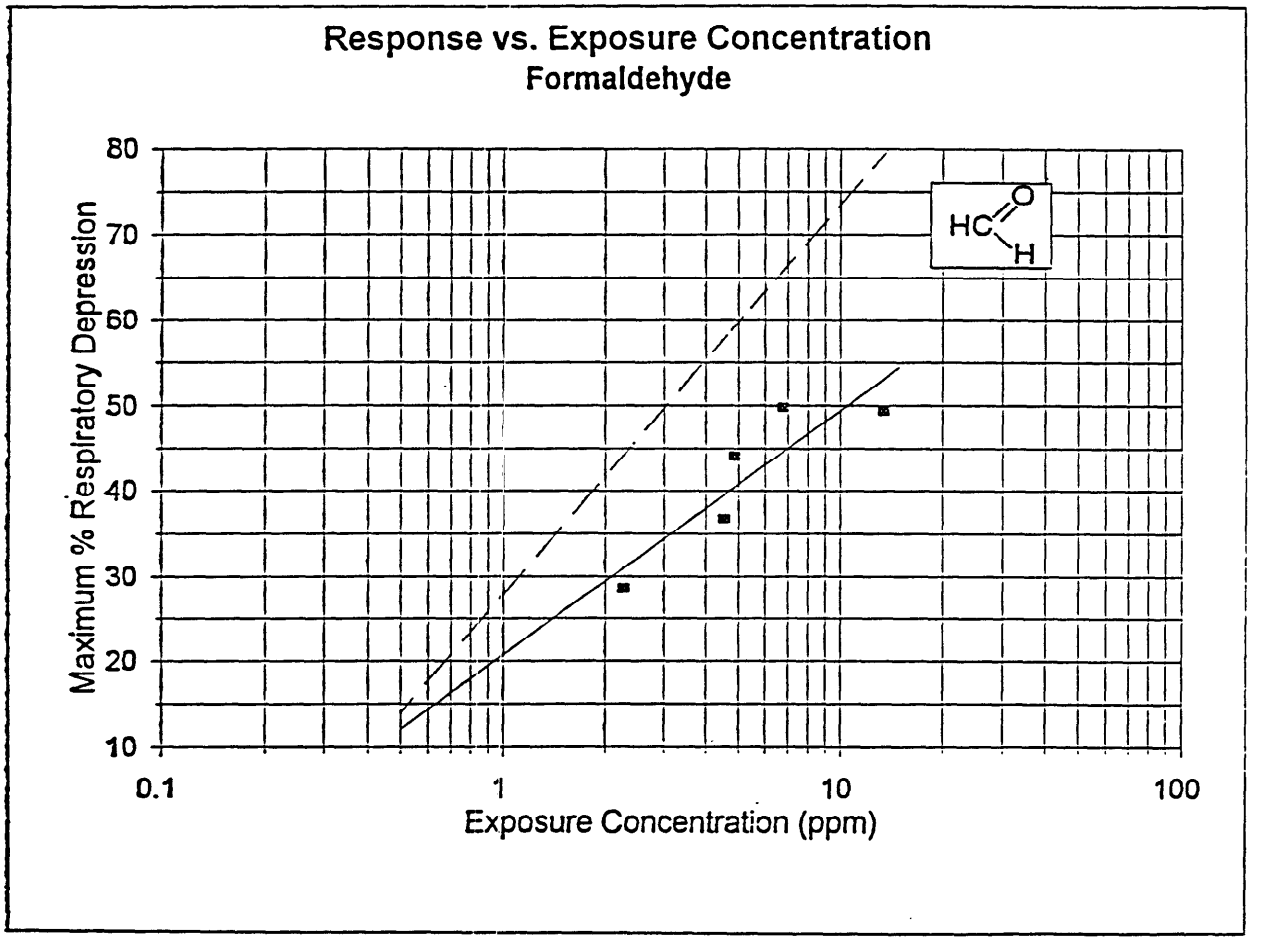

Response vs. Exposure Concentration
Formaldehyde
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
1
10
100
Exposure Concentration (mg/m3)
HC
O
H

FIGURE 31


Response vs. Exposure Concentration
Formaldehyde
Maximum % Respiratory Depression
80
70
60
50
40
30
20
10
0.1
1
10
100
Exposure Concentration (ppm)
HC
O
H

APPENDIX A

TOXICOLOGICAL INFORMATION FOR TARGET COMPOUNDS

TABLE OF CONTENTS

	Page Number
1,2,3-Trichloropropane	A-1
N,N-Dimethylacrylamide	A-5
1,4-Dimethylpiperazine	A-6
N,N-Dimethylbenzylamine	A-7
N,N-Dimethylacetamide	A-8
2-Methyleneglutaronitrile	A-17
2,6-Di-*tert*-butyl-4-methylphenol	A-18
Benzothiazole	A-20
2-Ethylhexanoic acid	A-21
4-Phenylcyclohexene	A-24
1,3-Dichloro-2-propanol	A-25
1-Dodecanol	A-26
ε-Caprolactam	A-27
Limonene (Dipentene)	A-30
2-Methylnaphthalene	A-37
Adiponitrile	A-38
Octamethylcyclotetrasiloxane	A-42
Nonanal	A-44
Phenyl Ether	A-45
2-Phenylphenol	A-47
Decamethylcyclopentasiloxane	A-51
Vinyl acetate	A-52
N,N-Dimethylformamide	A-61
1-Dodecene	A-65

2-Methylpropene A-69

Allyl Benzene A-70

Benzyl acetate A-71

2,2,4-Trimethyl-1,3-pentanediol diisobutyrate A-75

1,2,3-Trichloropropane

NAME OF SUBSTANCE 1,2,3-TRICHLOROPROPANE
CAS REGISTRY NUMBER 96-18-4

NON-HUMAN TOXICITY EXCERPTS
STRUCTURAL & ENZYMIC CHANGES WERE OBSERVED IN RAT LIVER FOLLOWING INHALATION OF 1,2,3-TRICHLOROPROPANE. SIGNIFICANT MORPHOLOGICAL & FUNCTIONAL CHANGES WERE OBSERVED IN CENTRAL LOBULAR SECTIONS OF THE LIVER. [BONASHEVSKAYA TI ET AL; DEPOSITED DOC (VINITI): 3169-76 (1976)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
EXPOSURE OF RATS AND GUINEA PIGS (5 OF EACH SEX) TO 800, 2100, OR 5000 PPM 1,2,3-TRICHLOROPROPANE FOR 30 MIN RESULTED IN CNS DEPRESSION, WHICH WAS MINIMAL @ 800 PPM BUT PROGRESSED TO ... /FURTHER CNS DEPRESSION/ & CONVULSIONS @ THE HIGHER CONCN. 2 OF 10 RATS & 6 OF 10 GUINEA PIGS DIED FOLLOWING EXPOSURE @ 5000 PPM; THE ONLY HISTOPATHOLOGIC LESION OBSERVED @ 14 DAYS POST-EXPOSURE WAS ADRENAL CORTICO-MEDULLARY NECROSIS. MORTALITY IN THE OTHER TWO EXPOSURE GROUPS WAS LIMITED TO 1 MALE RAT EXPOSED @ 2100 PPM; NO IRREVERSIBLE ORGAN LESIONS WERE REPORTED. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
EXPOSURE @ 30 MG/L (5000 PPM) FOR 20 MIN KILLED SEVERAL MICE, SOME DYING SEVERAL DAYS LATER FROM LIVER DAMAGE. DAILY 10-MIN EXPOSURES @ 2500 PPM FOR 10 DAYS RESULTED IN 7 DEATHS AMONG 10 MICE. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
ANESTHETIZED DOGS, RATS, MICE, MONKEYS, HAMSTERS AND RABBITS EXPOSED TO CONCN RANGING FROM 5,000-150,000 PPM HAVE SHOWN VARIOUS CARDIOVASCULAR & CIRCULATORY ABNORMALITIES. [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values, 4th ed., 1980. Cincinnati, Ohio: American Conference of Governmmental Industrial Hygienists, Inc., 1980. , p. 410] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
DOMINANT LETHAL STUDIES WERE CONDUCTED IN SPRAGUE-DAWLEY MALE RATS WITH 5 HALOGENATED 3-CARBON COMPOUNDS THAT ARE STRUCTURALLY SIMILAR TO A KNOWN MUTAGEN 1,2-DIBROMO-3-CHLOROPROPANE (DBCP). 15 MALES IN EACH GROUP WERE ADMINISTERED 1,2,3-TRICHLOROPROPANE BY GASTRIC INTUBATION ONCE A DAY FOR 5 SUCCESSIVE DAYS AT 80 MG/KG/DAY. 1,2,3-TRICHLOROPROPANE PRODUCED NEGATIVE RESPONSES FOR INDUCTION OF DOMINANT LETHALS. [SAITO-SUZUKI R ET AL; MUTAT RES 101 (4): 321-8 (1982)] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS
THE PRESENCE OF A DOUBLE BOND IN THE CASE OF 1,2,3-TRICHLOROPROPENE RESULTED IN A HIGHER LEVEL OF DIRECT MUTAGENIC ACTIVITY THAN 1,2,3-TRICHLOROPROPANE, BUT ACTIVATION WITH S-9 RESULTED IN A FURTHER INCREASE IN MUTAGENIC ACTIVITY OF SALMONELLA TYPHIMURIUM STRAIN TA100 WITH THE FORMER CMPD. [STOLZENBERG SJ, HINE CH; ENVIRON MUTAGEN 2 (1): 59-66 (1980)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
1,2,3-TRICHLOROPROPANE DID NOT PRODUCE PEROXIDATION OF MICROSOMAL LIPIDS AFTER MALE SPRAGUE-DAWLEY RATS RECEIVED A SINGLE INTRAGASTRIC DOSE OF 180 MG/KG. HEPATIC MICROSOMES SHOWED SIGNIFICANT DECREASE IN CYTOCHROME P-450 (& TO A LESSER EXTENT IN CYTOCHROME B5), & A SHIFT IN THE COMPOSITION OF MICROSOMAL FATTY ACID, PRIMARILY CHARACTERIZED BY A DECREASE IN ARACHIDONIC ACID & AN INCREASE IN LINOLEIC ACID. [MOODY DE ET AL; MOL PHARMACOL 20 (3): 685-93 (1981)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
INHALATION OF 0.002-2.2 MG 1,2,3-TRICHLOROPROPANE/L BY RATS FOR 1 DAY TO 3 MONTHS CAUSED MORE POLYPLOIDY OF THE HEPATOCYTE NUCLEI THAN DID 1,2-DICHLOROPROPANE. WITH DECREASING CONCN LONGER INHALATION PERIODS WERE REQUIRED FOR OBTAINING SIMILAR EFFECTS. [BELYAEVA NN ET AL; BYULL EKSP BIOL MED 83 (3): 345-8 (1977)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
CONTINUOUS INHALATION OF 0.4 & 0.8 MG/CU M OF 1,2,3-TRICHLOROPROPANE FOR 7 DAYS CAUSED HEMORRHAGES IN RAT LUNGS WITH DESQUAMATION & DESTRUCTION OF BRONCHIAL, BRONCHIOLAR & ALVEOLAR EPITHELIUM. SYMPTOMS WERE MILDER IN COMPARISON WITH 1,2-DICHLOROPROPANE. [BONASHEVSKAYA TI ET AL; DEPOSITED DOC (VINITI): 1733-78 (1978)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
FOLLOWING INCUBATION OF 1,2,3-TRICHLOROPROPANE, NADPH, EDTA, & HEPATIC MICROSOMES FROM PHENOBARBITAL-INDUCED RATS, DECREASES IN THE LEVELS OF CYTOCHROME P450, BUT NOT CYTOCHROME B5 OR NADPH-CYTOCHROME C REDUCTASE WERE NOTED. MICROSOMAL HEME DECREASED BY 60-100% OF THE DECREASE IN THE LEVELS OF CYTOCHROME P450, INDICATING THAT 1,2,3-TRICHLOROPROPANE DEGRADED THE HEME MOIETY OF CYTOCHROME P450. [IVANETICH KM ET AL; DRUG METAB DISPOS 6 (3): 218-25 (1978)] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS
Groups of 6 rats and mice were given single 4 hr exposures to vapor concn of 0, 125, 340, 700, or 2150 ppm 1,2,3-trichloropropane. All rats and mice exposed to 700 or 2150 ppm died, as did mice exposed to 340 ppm. There were clinical signs of labored respiration, inactivity, and eye and nasal irritation. These signs were observed to a lesser degree at 125 ppm. Except for a 10% weight loss, there appeared to be little specific injury, even in animals receiving a gross autopsy following exposure. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**
NON-HUMAN TOXICITY EXCERPTS

In a 120 day prechronic study, Fischer 344 rats were gavaged with corn oil soln of 1,2,3-trichloropropane. Daily doses were 0, 8, 16, 32, 63, 125 and 250 mg/kg body wt. Both sexes had 100% survival at 63 mg/kg. At 125 mg/kg, 18/19 males survived at 60 days and 9/9 at 120 days; 18/20 females survived at 60 days and 7/9 at 120 days. All rats of both sexes fed 250 mg/kg/day died in the first 60 days. There was a loss of body wt at 63 mg/kg/day but not at lower dosages. Clinical signs included thinness, hunched appearance, depression, and abnormal eye and urine stains at 125 and 250 mg/kg/day in both sexes and at 63 mg/kg/day in females only. ... One fourth of the animals sacrificed in a moribund condition had mottled livers at 250 mg/kg/day, as well as irritation of the glandular portion of the stomach and darkening and reddening of the renal medulla. Liver and liver-to-body wt ratios were increased in the 32, 63, and 125 mg/kg rat groups and in the 16, 32, 63, and 125 mg/kg female rat groups. Kidney and kidney-to-body wt ratios were increased in both sexes at 63 and 125 mg/kg/day. ... /Other/ gross observations included ... necrosis and inflammation of the nasal mucosa. Such changes were questionable at 32 mg/kg/day, but statistically significant at 63 and 125 mg/kg. Hematological changes, depressed rbc and hematocrit, were consistent with the injury to the liver and kidneys although even doses of 16 mg/kg resulted in depression. Clinical chemical changes were observed only at the highest dosage, but ... testicular weight, sperm count and sperm morphology showed no dose related effect in male rats. Groups of F6C3F1 mice appeared to respond similarly but to a slightly lesser degree. In both sexes, 19/20 survived 63 mg/kg/day for 60 days and 10/10 survived 120 days. Animals exposed to 32 mg/kg/day appear to be unaffected but the liver, kidneys, gastric mucosa and nasal passages were affected at higher levels. Sperm count appeared to be depressed at 125 and 250 mg/kg but testicular wt, epididymal wt, and sperm morphology were unaffected, suggesting a nonspecific secondary effect on the testes. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

15 daily doses of 37 mg/kg were given by ip injection to pregnant Sprague Dawley rats beginning on day 1 and ending on day 15 of pregnancy. There were no fetotoxic or teratogenic effects in the offspring, but maternal toxicity was reported in the dams. Male Sprague Dawley rats given 5 gavaged doses of 80 mg/kg/day showed no dominant lethal or testicular effects. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 602] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

In rats, vapors of 1,2,3-trichloropropane were more toxic than 1,1,1-trichloropropane. In one trial, 1000 ppm produced death in 5 of 6 rats after 4 hr of exposure; 1,1,1-trichloropropane at 8,000 ppm was required to produce similar results. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

1,2,3-trichloropropane was reported as nonirritating to intact and uncovered skin, but highly irritating to the eyes of rabbits. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed.

Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

1,2,3-Trichloropropane was the most toxic of 18 chlorinated alkyl hydrocarbons tested in dogs. Three dogs were fasted for 12 hr prior to intragastric admin. One dog received 0.2 ml/kg, one received 0.3 ml/kg, and one received 0.5 ml/kg. All three ... /had CNS depression/ within 1-2 hr and died within 1-2 days. Microscopic examination of the livers revealed fatty vacuolization and centrilobular necrosis. Cloudy swelling, desquamation of the tubular epithelium, and nuclear changes indicative of beginning necrosis were observed in the kidneys. [National Research Council. Drinking Water and Health, Volume 6. Washington, D.C.: National Academy Press, 1986. , p. 330] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

Spectrograde (99% pure) 1,2,3-trichloropropane produced liver damage in male CD1 rats. Rats that inhaled 500 ppm concn of the chemical for 4 hr exhibited increased levels of SGOT, SGPT, and ornithine carbamyl transferase 24 and 48 hr after exposure. [National Research Council. Drinking Water and Health, Volume 6. Washington, D.C.: National Academy Press, 1986. , p. 330] **PEER REVIEWED**

NON-HUMAN TOXICITY EXCERPTS

1,2,3-Trichloropropane was found to be active in 3 of 4 genetic toxicity testing categories: mutagenesis in Salmonella, chromosomal effects, transformation, and DNA damage. It did not induce detectable DNA damage in either the in vivo or in vitro unscheduled DNA synthesis V(DS) rat hepatocyte assay. [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 602] **PEER REVIEWED**

NON-HUMAN TOXICITY VALUES

LD50 Rat oral 450 mg/kg [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**

NON-HUMAN TOXICITY VALUES

LD50 Rabbit percutaneous 2500 mg/kg [American Conference of Governmental Industrial Hygienists. Documentation of the Threshold Limit Values and Biological Exposure Indices. 5th ed. Cincinnati, OH: American Conference of Governmental Industrial Hygienists, 1986. , p. 601] **PEER REVIEWED**