AKZO NOBEL

Safety,
Health,
Environmental,
and
Regulatory
Affairs

EDTN
HPV Robust Summaries
Akzo Nobel Functional Chemicals LLC
December 2002
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Akzo Nobel Chemicals, Inc.
5 Livingstone Avenue
Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

Akzo Nobel Chemicals, Inc.
5 Livingstone Avenue
Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

1. Substance Information

CAS Number:	5766-67-6
Chemical Name:	Acetonitrile, 2, 2', 2'', 2'''-(1,2-ethanediyldinitrilo) tetrakis-
Structural Formula:	C10H12N6
Other Names:	Acetonitrile, (ethylenedinitrilo) tetra-; EDTN
Exposure Limits:	None

2. Physical – Chemical Properties

2.1. Melting Point:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 102
GLP:	Yes
Year:	1998
Value:	73-74°C
Decomposition:	At temperatures above 231°C
Conclusions:	The melting point of PDTN is 73-74°C.
Reliability:	1
Reference:	[1]
Remarks:	None
Additional References for Melting Point Studies:	None

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Value:	159°C
Decomposition:	Not available
Conclusions:	The melting point of EDTN is estimated to be 159°C.
Reliability:	1
Reference:	[2]

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Remarks:	None
Additional References for Melting Point Studies:	None

2.2. Boiling Point:

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Value:	427.17°C
Decomposition:	Not available
Conclusions:	The boiling point of EDTN is estimated to be 427.17°C.
Reliability:	1
Reference:	[3]
Remarks:	None
Additional References for Melting Point Studies:	None

2.3. Density:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 109
GLP:	Yes
Year:	1998
Value:	1.23 g/cm^3
Conclusions:	The density of PDTN is 1.23 g/cm^3.
Reliability:	1
Reference:	[4]
Remarks:	None
Additional References for Density Studies:	None

2.4. Vapor Pressure:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN

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	99.2%; other test substance; analog PDTN
Method:	OECD 104
GLP:	Yes
Year:	1998
Value:	0.19±2 Pa = 1.43±0.15 x 10^{-3} mmHg
Temperature° C:	20
Pressure Unit:	Pa or mmHg
Decomposition:	No
Conclusions:	The vapor pressure of PDTN at 20°C is 0.19±2 Pa = 1.43±0.15 x 10^{-3} mmHg.
Reliability:	1
Reference:	[5]
Remarks:	Static technique was used in the study
Additional Reference for Vapor Pressure Studies:	None

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Value:	7.54 x 10^{-8} mmHg
Temperature° C:	25
Pressure Unit:	Mm Hg
Decomposition:	Not available
Conclusions:	The vapor pressure of EDTN at 25°C is estimated to be 7.54 x 10^{-8} mmHg.
Reliability:	1
Reference:	[6]
Remarks:	None
Additional Reference for Vapor Pressure Studies:	None

2.5. Partition Coefficient (log Kow):

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN

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Method:	107
GLP:	Yes
Year:	1998
Log Kow:	-1.3
Temperature°C:	40
Conclusions:	The log Kow of PDTN is –1.3.
Reliability:	1
Reference:	[7]
Remarks:	None
Additional References for Partition Coefficient Studies:	None

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Log Kow:	-2.17
Temperature°C:	Not available
Conclusions:	The log Kow of EDTN is estimated to be –2.17.
Reliability:	1
Reference:	[8]
Remarks:	None
Additional References for Partition Coefficient Studies:	None

2.6. Water Solubility:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	105
GLP:	Yes
Year:	1998
Value at temperature°C:	1.67g/L at 18±1.5°C

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Phone: 914-674-5000
Fax: 914-693-0836

Description of solubility:	Clear
PH value and concentration at temperature °C:	7.8-8.1 at 18±1.5°C
Pka value at 25°C:	Not reported
Conclusions:	The water solubility of PDTN is 1.67 g/L.
Reliability:	1
Reference:	[9]
Remarks:	None
Additional References for Water Solubility Studies:	None

Identity:	EDTN; CAS# 576-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Year:	Not applicable
Value at temperature°C:	1000 g/L at 25°C
Description of solubility:	Not available
PH value and concentration at temperature °C:	Not available
Pka value at 25°C:	Not available
Conclusions:	The water solubility of EDTN is estimated to be 1000 g/L.
Reliability:	1
Reference:	[10]
Remarks:	None
Additional References for Water Solubility Studies:	None

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5 Livingstone Avenue
Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

3. Environmental Fate

3.1. Photodegradation:

Identity:	EDTN; CAS# 5766-67-6
Method:	EPIWIN Computer Model
GLP:	Not applicable
Type:	Not applicable
Year:	Not applicable
Light Source:	Not applicable
Light Spectrum (nm):	Not applicable
Half-life:	4.589 hours
Breakdown Products:	Not available
Conclusions:	The half-life in the atmosphere for EDTN is estimated to be 4.589 hours.
Reference:	[11]
Remarks:	None
Additional References for Photodegradation Studies:	None

3.2. Stability in Water:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	EEC Directive 92/69, Part C Publication L383 1992
GLP:	Yes
Type:	Hydrolysis as a function of pH
Year:	1999
Half-life at a specific pH:	pH 4: 5.3 years at 25°C pH 7: 3.9 years at 25°C pH 9: 0.3 years at 25°C
Breakdown Products:	Not determined
Conclusions:	The half-life of PDTN at pH 4, 7 and 9 at 25°C is 5.3, 3.9 and 0.3 years, respectively.
Reliability:	1
Reference:	[12]
Remarks:	Half-life at 25°C estimated from data of studies at higher temperatures.

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Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

Additional References for Stability in Water Studies:	None

3.3. Transport (Fugacity):

Identity:	EDTN; CAS# 5766-67-6			
Method:	EPIWIN Computer Model			
GLP:	Not applicable			
Type:	Not applicable			
Year:	Not applicable			
Media:	Air, Water, Soil, Sediment			
Distributions:	Compartment	Released 100% to air	Release 100% to water	Release 100% to soil
	Air	3.99×10^{-14}	3.3×10^{-31}	7.07×10^{-29}
	Water	39.8	99.8	36
	Soil	60.2	4.98×10^{-16}	64
	Sediment	0.0753	0.189	0.0681
Conclusions:	EDTN is distributed primarily to water and soil.			
Reliability:	1			
Reference:	[13]			
Remarks:	When released equally to air, water and soil, EDTN is distributed 51.8% to water and 48.1% to soil.			
Additional References for Transport (Fugacity) Studies:	None			

3.4. Biodegradation:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 301
Type:	Modified Sturm Test
GLP:	Yes
Year:	1998
Degradation% after time:	0% at 28 days
Breakdown Products:	Not determined
Concentration Of Test Chemical:	12 mg TOC/L
pH Of Test Media:	7.8-8.1
Conclusions:	PDTN is not readily biodegradable.

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Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

Reliability:	1
Reference:	[14]
Remarks:	Source of test organism was activated sludge obtained from a municipal sewage treatment plant
Additional References for Biodegradation Studies:	None

4. Ecotoxicity

4.1. Acute Toxicity to Fish:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	203
Type:	Static
GLP:	Yes
Year:	1998
Species/Strain:	Zebra fish/Teleostie, Cyprinidae
Supplier:	Charles River Aquatics, The Netherlands
Analytical Monitoring:	Gas Chromatography
Exposure Period:	96 hours
Nominal/Measured Concentrations:	100 mg/L; 107-109 mg/L
LC50:	>100 mg/L
Conclusions:	The LC50 of PDTN in zebra fish is >100 mg/L.
Reliability:	1
Reference:	[15]
Remarks:	There was no mortality during the study. Ten fish were used in the test group. The water hardness was 250 mg/CaCO3/L. The pH was 7.2-8.2. The temperature was 20.7-21.3°C. The DO was 4.7-9.
Additional References for Acute Toxicity to Fish Studies:	None

4.2. Acute Toxicity to Invertebrates:.

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	202
Type:	Static
GLP:	Yes

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Phone: 914-674-5000
Fax: 914-693-0836

Year:	1998
Species/Strain	Daphnia magna/Crustacea, Cladocera Strauss, 1820
Supplier:	Not available
Analytical Monitoring:	Gas Chromatography
Exposure Period:	48 hours
Nominal/Measured Concentrations:	1, 10, 100 mg/L; 110 mg/L
EC50:	>100 mg/L
Conclusions:	The EC50 of PDTN in Daphnia magna is >100 mg/L.
Reliability:	1
Reference:	[16]
Remarks:	There was no mortality during the study. Ten fish were used at 1 and 10 mg/L and 20 fish in the 100 mg/L group. The water hardness was 250 mg/CaCO3/L. The pH was 8.0-8.3. The temperature was 21.0-21.3°C. The DO was 8.8-8.9.
Additional References for Acute Toxicity to Invertebrates Studies:	None

4.3. Acute Toxicity to Aquatic Plants:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	201
Type:	Growth Inhibition Test
GLP:	Yes
Year:	1998
Species/Strain/ Supplier:	Selenastrum capricornutum/CCAP 278/4/Not avialable
Analytical Monitoring:	Gas Chromatography
Exposure Period:	72 hours
Nominal/Measured Concentrations:	10, 18, 32, 56, 100 and 180 mg/L/10.5, 34, 189
EC50:	Growth inhibition – 60 mg/L; Growth rate reduction – 129 mg/L
Conclusions:	The EC50 in algae for growth inhibition and growth rate reduction for PDTN is 60 and 129 mg/L, respectively.
Reliability:	1
Reference:	[17]

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Remarks:	Three replicates of the test concentrations were done. The water hardness was Ca+Mg: 0.24 mmol/L (24 mg CaCo3/L). The pH was 8.1-8.4. The temperature was 21.2-23.0°C. The DO was 8.8-8.9.
Additional References for Acute Toxicity to Aquatic Plants Studies:	None

5. Mammalian Toxicity

5.1. Acute Toxicity:

5.1.1. Oral

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 423
Type:	Acute Toxic Class Method
GLP:	Yes
Year:	1998
Species/Strain:	Rat/Wistar Cr1(WI)
Sex:	M/F
No. Of Animals Per Sex Per Dose:	3
Vehicle:	Polyethylene glycol
Route Of Administration:	Oral gavage
Time Of Observation Period:	15 Days
Doses Administered:	2000 mg/kg
LD50:	>2000 mg/kg
Conclusions:	The oral LD50 of PDTN in rats is greater than 2000 mg/kg.
Reliability:	1
Reference:	[18]
Remarks:	One female was found dead on day 3. Clinical signs of toxicity were lethargy, hunched posture, piloerection, diarrhea and red staining of the snout between days 1 and 3. Macroscopic examination showed hemorrhagic content of the urinary bladder in the animal that died. There were no effects in surviving animals.

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5 Livingstone Avenue
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Phone: 914-674-5000
Fax: 914-693-0836

Additional References for Acute Oral Toxicity Studies:	None

5.1.2. Dermal

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 402
Type:	Acute Dermal
GLP:	Yes
Year:	1998
Species/Strain:	Rat/Wistar Cr1(WI)
Sex:	M/F
No. Of Animals Per Sex Per Dose:	5
Vehicle:	Polyethylene glycol
Route Of Administration:	Dermal
Time Of Observation Period:	15 Days
Doses Administered:	2000 mg/kg for 24 hours
LD50:	>2000 mg/kg
Conclusions:	The dermal LD50 of PDTN in rats is greater than 2000 mg/kg.
Reliability:	1
Reference:	[19]
Remarks:	There was no mortality. Clinical signs of toxicity were red staining of the neck in one female between days 3 and 7 and scabs or scales in the treated area of two other females between days 3 and 6. Macroscopic examination showed no abnormalities.
Additional References for Acute Dermal Toxicity Studies:	None

5.1.3. Skin Irritation

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 404
Type:	Semi-Occlusive

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Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

GLP:	Yes
Year:	1998
Species/Strain:	Rabbit/New Zealand white
Sex:	M
No. Of Animals:	3
Vehicle:	Water
Route Of Administration:	Dermal
Time Of Exposure:	4 hours
Time Of Observation Period:	1, 24, 48 and 72 hours
Concentration Of Test Material:	0.5g
Results:	There was no erythema or edema at any observation period.
Conclusions:	PDTN was not irritating to rabbits following dermal exposure for 4 hours.
Reliability:	1
Reference:	[20]
Remarks:	None
Additional References for Acute Dermal Irritation Studies:	None

5.1.4. Sensitization

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 406
Type:	Maximization Test
GLP:	Yes
Year:	1998
Species/Strain:	Guinea Pig/Dunkin Hartley
Sex:	F
No. Of Animals:	10
Vehicle:	Corn Oil
Route Of Administration:	Dermal
Time Of Observation Period:	24 Days
Concentration Of Test Material:	Induction: Day 1 – 0.1%; Day 8 – 50%; Challenge: Day 21 – 50%
Results:	There was no irritation seen 24 or 48 hours after challenge application.

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Phone: 914-674-5000
Fax: 914-693-0836

Conclusions:	PDTN was not sensitizing to guinea pigs at a 50% challenge concentration.
Reliability:	1
Reference:	[21]
Remarks:	Alpha-hexylcinnamic aldehyde was the positive control.
Additional References for Acute Dermal Sensitization Studies:	None

5.2. Repeated Dose Toxicity:

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 407
Type:	28-Day Oral Toxicity
GLP:	Yes
Year:	1998
Species/Strain:	Rat/Wistar Cr1(WI)BR
Sex:	M/F
No. Of Animals Per Sex Per Dose:	20
Vehicle:	Polyethylene glycol
Route of Administration:	Oral gavage
Time of Observation Period:	28 Days
Doses Administered:	50, 200,1000 mg/kg/day
Frequency of Treatment:	Once daily for 28 days, 7 days per week
NOAEL (NOEL):	200 mg/kg
LOAEL (LOEL):	1000 mg/kg
Toxic Response By Dose Level:	1000 mg/kg: Mortality – one female on day 23; Clinical signs – piloerection, hunched posture, severe brown staining of the fur, red discoloration of the urine of females; Clinical chemistry – Significant increase in alanine aminotransferase activity of males and females; Macroscopic exam - enlarged kidney and urinary bladder in female that died during the study; Organ weights – a minor significant increase in liver to body weight ration in males at 1000 mg/kg/day; Microscopic exam – minimal to slight centrilobular hepatocellular hypertrophy in males and females at 1000 mg/kg/day, female that died during the study had marked

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	mg/kg/day, female that died during the study had marked hydronephrosis, moderate tubular dilation and pyelonephritis and moderate inflammation of the urinary bladder. 200 mg/kg/day: Clinical signs – severe brown staining of the fur. 50 mg/kg/day: None
Conclusions:	PDTN administered daily by oral gavage to rats for 28 days resulted in signs of liver toxicity at 1000 mg/kg/day. The effects on the liver included an increased liver weight and alanine aminotransferase activity and microscopic changes. The NOAEL was 200 mg/kg/day.
Reliability:	1
Reference:	[22]
Remarks:	None
Additional References for Repeated Dose Toxicity Studies:	None

5.3. Genetic Toxicity:

5.3.1. *In Vitro* Gene Mutations

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 471/472
Type:	Ames Test
GLP:	Yes
Year:	1998
Cell Type:	Salmonella typhimurium TA1535, TA1537, TA98, TA100; E.coli WP2uvrA
Metabolic Activation:	Rat S9 induced by Aroclor 1254
Concentrations Tested:	Without S9:3, 10, 33, 100, 333, 1000, 3330, 5000 With S9: 100, 333, 1000, 3330, 5000
Vehicle:	Dimethyl sulfoxide
Cytotoxic Concentration:	No toxicity at any concentration.
Genotoxic Effects With Metabolic Activation:	None
Genotoxic Effects Without Metabolic Activation:	None
Conclusions:	PDTN was not mutagenic in Salmonella typhimurium strains TA1535, TA1537, TA98, TA100 or E.coli strain WP2uvrA in the presence or absence of metabolic activation.

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Phone: 914-674-5000
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Reliability:	1
Reference:	[23]
Remarks:	The test concentrations were tested in triplicate.
Additional References for In Vitro Gene Mutation Studies:	None

5.3.2. *In Vitro* Chromosome Aberrations

Identity:	PDTN; CAS# 110057-45-9; Batch JNN98038; purity – 99.2%; other test substance; analog PDTN
Method:	OECD 473
Type:	In Vitro
GLP:	Yes
Year:	1998
Cell Type:	Cultured peripheral human lymphocytes
Metabolic Activation	Rat S9 induced by Aroclor 1254
Concentrations Tested:	Without S9: 333, 1000, 3330 (24 and 48 hour treatment) With S9: 100, 333, 1000, 3330, 5000 (3 hour treatment)
Vehicle:	Dimethylsulfoxide
Cytotoxic Concentration:	No toxicity at any concentration.
Genotoxic Effects With Metabolic Activation:	None
Genotoxic Effects Without Metabolic Activation:	None
Conclusions:	PDTN was not clastogenic in cultured peripheral human lymphocytes in the presence and absence of metabolic activation.
Reliability:	1
Reference:	[24]
Remarks:	The test concentrations were tested in duplicate.
Additional References for *In Vitro* Chromosome Aberration Studies:	None

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Phone: 914-674-5000
Fax: 914-693-0836

References

1 Determination Of The Melting Temperature Of PDTN. NOTOX Project No. 234822 11/19/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

2 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

3 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

4 Determination Of The Density Of PDTN. NOTOX Project No. 234844 10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

5 Determination Of The Vapour Pressure Of PDTN. NOTOX Project No. 234855 10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

6 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

7 Determination Of The Partition Coefficient (N-Octanol/Water) Of PDTN. NOTOX Project No. 234855 10/21/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

8 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

9 Determination Of The Water Solubility Of PDTN. NOTOX Project No. 234877 11/2/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

10 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

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Dobbs Ferry, NY 10522-3407
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Fax: 914-693-0836

11 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

12 Determination Of The Hydrolysis Of PDTN As A Function Of pH.
NOTOX Project No. 258582 4/9/99. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

13 EPIWIN 3.10 U.S. Environmental Protection Agency 2000

14 Determination Of 'Ready' Biodegradability: Carbon Dioxide (CO_2) Evolution Test
(Modified Sturm Test) With PDTN. NOTOX Project No. 235057 9/11/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

15 96-Hour Acute Toxicity Study In Zebra-Fish With PDTN (Static).
NOTOX Project No. 235068 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

16 Acute Toxicity Study In Daphnia Magna With PDTN (Static).
NOTOX Project No. 235079 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

17 Fresh Water Algal Growth Inhibition Test With PDTN.
NOTOX Project No. 235081 10/29/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

18 Assessment Of Acute Oral Toxicity With PDTN In The Rat (Acute Toxic Class Method).
NOTOX Project No. 234967 9/23/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

19 Assessment Of Acute Dermal Toxicity With PDTN In The Rat.
NOTOX Project No. 234978 9/23/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

20 Primary Skin Irritation/Corrosion Study With PDTN In The Rabbit
(4-Hour Semi-Occlusive Application). NOTOX Project No. 234989 9/23/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

21 Assessment Of Contact Hypersensitivity To PDTN In The Albino Guinea Pig (Maximization-Test).
NOTOX Project No. 235002 10/26/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

22 Subacute 28-Day Oral Toxicity With PDTN By Oral Gavage In The Rat.
NOTOX Project No. 235024 11/19/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

23 Evaluation Of The Mutagenic Activity Of PDTN In The Salmonella Typhimurium Reverse
Mutation Assay And the Eschiricia Coli Reverse Mutation Assay (With Independent Repeat).
NOTOX Project No. 235035 9/7/98. Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

24 Evaluation Of The Ability Of PDTN To Induce Chromosome Aberrations In Cultured
Peripheral Human Lymphocytes. NOTOX Project No. 235046 10/30/98.
Sponsor: Akzo Nobel Chemicals B.V. The Netherlands

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5 Livingstone Avenue
Dobbs Ferry, NY 10522-3407
Phone: 914-674-5000
Fax: 914-693-0836

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5 Livingstone Avenue
Dobbs Ferry, NY 10522-3407
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Fax: 914-693-0836