STRUCTURE-ACTIVITY TEAM REPORT [redacted]

PMN:	P-95-0979, 980 + 981	DCN:	
SAT Date:	4/14/95	SAT Chair:	V. Nabholz

95 JUN -9 AM 10: 02

Submitter: E. I. DuPont

Chemical Name:

[redacted]

50950005483

CAS RN:	[redacted]	Trade Name:	[redacted]

Structure: [redacted]

Formula:	[redacted]		
Mol Weight:	[redacted]	WT%<500:	WT%<1000:
MP:	BP:		Eq Wt:
H2O Sol (g/L):	Dispersive	VP:	< 0.000001
Physical State:	[redacted]		
Max Prod Volume (kg/yr):	[redacted]	Other:	

Use:
Chemical intermediate [redacted]

Related Case Number	Case Role	Related Case Number	Case Role
[redacted]			

FOCUS	Date: APR 20 1995	Results:	NON SE SNUR

STRUCTURE-ACTIVITY TEAM REPORT [redacted]	
PMN: P-95-0980	DCN:
SAT Date: 4/14/95	SAT Chair: V. Nabholz
Submitter: E. I. DuPont	
Chemical Name: [redacted]	
CAS RN: [redacted]	Trade Name: [redacted] NA
Structure: [redacted]	
Formula: [redacted]	
Mol Weight: [redacted]	WT%<500: / WT%<1000:
MP:	BP: / Eq Wt:
H2O Sol (g/L): Dispersive	VP: < 0.000001
Physical State: [redacted]	
Max Prod Volume (kg/yr): [redacted]	Other:
Use: [redacted]	

Related Case Number	Case Role	Related Case Number	Case Role
		[redacted]	

FOCUS	Date: APR 20 1995	Results: NON SE SNUR

STRUCTURE-ACTIVITY TEAM REPORT [redacted]	
PMN: P-95-0981	DCN:
SAT Date: 4/14/95	SAT Chair: V. Nabholz
Submitter: E. I. DuPont	
Chemical Name: [redacted] c [redacted]	
CAS RN: [redacted]	Trade Name: [redacted] NA
Structure: [redacted]	
Formula: [redacted]	
Mol Weight: [redacted]	WT%<500: / WT%<1000:
MP:	BP: / Eq Wt:
H2O Sol (g/L): Dispersive	VP: < 0.000001
Physical State: [redacted]	
Max Prod Volume (kg/yr): [redacted]	Other:
Use: Chemical intermediate [redacted]	

Related Case Number	Case Role	Related Case Number	Case Role

FOCUS	Date: APR 20 1995	Results: NON SE SNUR

STRUCTURE ACTIVITY TEAM REPORT 04-14-95 [redacted]

CASE NUMBERS: **P95-0979, 0980, and 0981**

RELATED CASES: [redacted] **0979:** [redacted] **0980:** [redacted] **0981:** [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:		HEALTH	ECOTOX
LEVEL OF CONCERN:	**0979**	2-3	2
	0980	2-3	2
	0981	2-3	3

KEYWORDS: LIVER, LUNG, DEVEL, UNCERT (SENS-CARDIAC, NEURO), AQUATOX (A,C)

SUMMARY OF ASSESSMENT:

FATE: Water solubility is dispersible; log K_{ow} = x.x (**0979**), x.x (**0980**), x.x (**0981**) via (CLOGP for free acid), and 3.7 (**0979**), 4.9 (**0980**), >7.0 (**0981**) via (SRC for free acid); low sorption; POTW removal = [redacted] vapor pressure < 10E-6 torr; ultimate biodegradation > months.

HEALTH: Absorption poor thru skin based on analogs; **0979** good thru GI, but **0980** and **0981** moderate thru GI based on analogs; and good thru lungs based on physical/chemical properties; submitted test data for an analog: [redacted] were rat acute oral LD ≥ 60 mg/kg and liver toxicity at 12 mg/kg; rabbit acute dermal ALD = 130 mg/kg; rat acute inhalation (6h/d/14d) test reported liver toxicity ≥ 5 ppb; rat 14-d oral toxicity test reported liver toxicity at 0.6 mg/kg/d; and dog acute oral reported liver toxicity at 4 mg/kg; concern for liver toxicity based on [redacted] concern for developmental toxicity based on [redacted]; concern for lung toxicity if inhaled due to surfactancy; uncertain concern for cardiac sensitization and neurotoxicity; no concern for oncogenicity;
moderate-high concern.
All exposures to humans: inhalation, dermal, ingestion, drinking water;

ECOTOX: **0979:** Predicted toxicity values are:

fish 96-h LC50	≤	200.0	mg/L
daphnid 48-h LC50	≤	30.0	mg/L
green algal 96-h EC50	≤	10.0	mg/L
fish Chronic Value (ChV)	≤	20.0	mg/L
daphnid ChV	≤	3.0	mg/L
algal ChV	≤	1.0	mg/L

based on SARs for [redacted]
pH 7, hardness <180.0 mg/L as $CaCO_3$;

moderate concern;
concern concentration (CC) = 0.100 [redacted]
[redacted]

0980: Predicted toxicity values are:

fish 96-h LC50	≤	60.0	mg/L
daphnid 48-h LC50	≤	3.0	mg/L
green algal 96-h EC50	≤	12.0	mg/L
fish Chronic Value (ChV)	≤	6.0	mg/L
daphnid ChV	≤	0.300	mg/L
algal ChV	≤	1.0	mg/L

based on SARs for [redacted]
pH 7, hardness <180.0 mg/L as $CaCO_3$;
moderate concern;
concern concentration (CC) = 0.030 mg/L.
[redacted]

0981: Predicted toxicity values are:

fish 96-h LC50	≤	11.0	mg/L
daphnid 48-h LC50	≤	0.300	mg/L
green algal 96-h EC50	≤	30.0	mg/L
fish Chronic Value (ChV)	≤	1.0	mg/L
daphnid ChV	≤	0.030	mg/L
algal ChV	≤	3.0	mg/L

based on SARs for [redacted]
pH 7, hardness <180.0 mg/L as $CaCO_3$;
high concern;
concern concentration (CC) = 0.003 mg/L.
[redacted]

Vince Nabholz [redacted]

BIOLOGICAL TEST INFORMATION

OECD Status: N

Reviewer Initials: Uc Case Number: P-95-979-981 Date Received: 3/28/95 Page: 1 of 2

This information is for: [redacted]

Study Type: Skin absorption Study Duration: Species/Sex: Rabbits

Wt/Life Stage: No. Groups/No. Per Group: Controls:

Route: Dose Range:

Characteristics of Tested Substance:

Test Conditions (Dosing Regimen):

Results: ALD = 130 mg/kg.

This information is for: [redacted]

Study Type: Oral Study Duration: Species/Sex: Rat (M)

Wt/Life Stage: No. Groups/No. Per Group: Controls:

Route: Dose Range:

Characteristics of Tested Substance:

Test Conditions (Dosing Regimen):

Results: Death occurred in males at dosages of 60 mg/kg or greater.

Comments: [redacted]

Genotoxicity data for [redacted]

[ ] AMES +/-(with/without activation) STRAIN if (+):
[ ] E. Coli Reverse Mutation +/-(with/without activation)
[ ] Chromosome Abs in CHO/CHL +/-(with/without activation)
[ ] Other:
[ ] Mouse Micronucleus +/- (ip/oral)
[ ] Rat Hepatocyte UDS +/-

Other Data: [ ] Ecotox [X] Fate [ ] Water Solubility/LogP % ai:

BIOLOGICAL TEST INFORMATION

OECD Status: N

Reviewer Initials: lic Case Number: P - 95-979-981 Date Received: 3/28/95 Page: 2 of 2

This information is [redacted]

Study Type: Inhalation [redacted] Species/Sex: Rats

Wt/Life Stage: No. Groups/No. Per Group: Controls:

Route: Dose Range: 5, 50 and 500 ppb

Characteristics of Tested Substance:

Test Conditions (Dosing Regimen): doses were given 6 hrs/day, five days/week for 2 weeks

Results: Histopathologic evaluations of the liver revealed changes characterized by swollen, eosinophilic hepatocytes which had a granular cytoplasm.

This information is for: [ ] Submitted Substance [ ] Analog:

Study Type: Study Duration: Species/Sex:

Wt/Life Stage: No. Groups/No. Per Group: Controls:

Route: Dose Range:

Characteristics of Tested Substance:

Test Conditions (Dosing Regimen):

Results:

Comments:

Genotoxicity data for: [ ] Submitted Substance [ ] Analog:

[ ] AMES +/-(with/without activation) STRAIN if (+):
[ ] E. Coli Reverse Mutation +/-(with/without activation)
[ ] Chromosome Abs in CHO/CHL +/-(with/without activation)
[ ] Other:
[ ] Mouse Micronucleus +/- (ip/oral)
[ ] Rat Hepatocyte UDS +/-

Other Data: [ ] Ecotox [ ] Fate [ ] Water Solubility/LogP % ai:

FEB SAT REPORT [redacted]	[redacted] Y/N):
PMN: P-95-0979	CAS RN: [redacted]
Chemical Name: [redacted]	Analogs:

Structure: [redacted]

Use: Chemical intermediate [redacted]

Formula:	[redacted]	Wt:	
Mol Weight: [redacted]	Wt%<500:		Wt%<1000
MP:	BP:		VP: < 0.000001
H2O Sol (g/L): Dispersive	Physical State: [redacted]		Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	200		
Daphnid 48-h	0.13		
Algal 96-h	10		
Fish ChV	30		
Daphnid ChV	0.02		
Algal ChV	5.0		
BCF			

CHEMICAL CLASS:				SAR: [redacted]	
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION	0.002
DATE 4-14-95				ASSESSOR: AK/GC	

EEB SAT REPORT [redacted]	(Y/N):
PMN: P-95-0980	CAS RN: [redacted]

Chemical Name:	Analogs:
[redacted]	

Structure:

[redacted]

Use: [redacted]

Formula:	[redacted]	t:	
Mol Weight: [redacted]	Wt%<500:		Wt%<1000
MP:	BP:		VP: < 0.000001
H2O Sol (g/L): Dispersive	Physical State:	Solid	Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	60.0		
Daphnid 48-h	0.03		
Algal 96-h	12.0		
Fish ChV	9.0		
Daphnid ChV	0.005		
Algal ChV	6.0		
BCF			

CHEMICAL CLASS:				SAR: [redacted]	
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION	0.001
DATE 4-14-95				ASSESSOR: AK/GC	

EEB SAT REPORT [redacted]

PMN: P-95-0981	CAS RN: [redacted]

Chemical Name: [redacted]

Analogs:

Structure: [redacted]

Use:

Chemical intermediate [redacted]

Formula:	[redacted]	Eq Wt:	
Mol Weight:	[redacted]	Wt%<500:	Wt%<1000
MP:		BP:	VP: < 0.000001
H2O Sol (g/L):	Dispersive	Physical State:	Solid Log P:

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	11.0		
Daphnid 48-h	0.007		
Algal 96-h	30.0		
Fish ChV	2.0		
Daphnid ChV	0.001		
Algal ChV	15.0		
BCF			

CHEMICAL CLASS:				SAR:	[redacted]
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION	0.001
DATE 4-14-95				ASSESSOR: AK/GC	

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE APR 14 1995

ATTENDEES	SIGNATURE
CHEMISTRY	
Paul Bickart	
Diana Darling	
Steve DeVito	
Fred Metz	
✓ JENNY TOU	Jenny Tou
ENVIRONMENTAL FATE	
Bob Boethling	
David Lynch	
✓ Gary Thom	GCThom
HEALTH	
Angela Auletta	
✓ Michael Cimino	Michael C Cimino
Fredrick Di Carlo	
✓ Leonard Keifer	L Keifer
David Lai	
✓ Jim Murphy	
✓ Deborah Norris	D. Norris
X Yin Tak Woo	X
ENVIRONMENTAL EFFECTS	
✓ Gordon Cash	Gordon Cash
Anne Kim	
Larry Newsome	
SAT CHARIPERSON/OTHER	
Rebecca Jones	
✓ Vince Nabholz	
Pauline Wagner	