[redacted] **Final** **FOCUS REPORT**
New Chemicals Program

[redacted]

PART I: BACKGROUND

Written By: DDH

FOCUS DATE: 6/24/04 **FOCUS CHAIR:** K. Moss

COMPANY: Champion Technologies

CASE NUMBER(S): P04-0625 **through** **and**

PART II: SAT RESULTS

HEALTH: 2 **ECOTOX:** 3 **OCCUPATIONAL EXPOSURE:** 1-2 **CONSUMER EXPOSURE:** 0-1 **ENVIRONMENTAL RELEASES:** 0-1

ADDITIONAL SAT INFORMATION:

PART III: OTHER FACTORS

a. **PRODUCTION VOLUME:** [redacted] kg/yr

5 0 0 4 0 0 0 4 3 6 4

b. **PROD VOL OTHER:**

c. **USE:** [redacted]

d. **REGULATORY HISTORY:** [redacted] WITHDRAWN/FACE 5E
FOCUS DROP
[redacted] REG NON 5E SNUR

e. **TEST DATA:**

f. **IMPORTED** ☐ **MANUFACTURED** ☑ **BOTH** ☐

g. **MSDS:** ☑

h. **CATEGORY:** Cationic Surfactants **CATEGORY 2:**

PART IV: SUMMARY OF SAT ASSESSMENT

CASE NUMBER: P04-0625

FATE [redacted]; Estimations for covalent ion pair
[redacted]; LogBCF = 1.85(E);
POTW removal(%)= 90 via sorption & [redacted]
Time for complete ultimate aerobic biodeg = wk
PBT Potential: P1B1T2
Sorption to soils/sediments = strong - v.strong

HEALTH: Absorption poor thru skin with irritation based on submitted test data for an analog, good thru lungs and moderate thru GI based on analogs. Concern for irritation and corrosion to all membranes from high ai products based on analog test data and [redacted]; neurotoxicity from the quaternary; lung toxicity if inhaled due to surfactancy for low ai products; developmental toxicity based on [redacted] (rat developmental toxicity NOEL = 50 mg/kg, delayed ossification at 100 mg/kg); and dermal sensitization from the quaternary nitrogen moiety.

test data for [redacted] were: rat acute oral LD50 = 600 mg/kg with effects to the lungs, liver, kidney, and GI tract irritation; severe skin irritation with corrosion in rabbits

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:
fish 96-h LC50 < 0.360 P

daphnid 48-h LC50 < 0.960 P
green algal 96-h EC50 < 0.690 P
fish Chronic Value (ChV) < 0.040 P
daphnid ChV < 0.100 P
algal ChV < 0.070 P
Predictions based on SARs for monoalkyl quaternary surfactants C16 and excess toxicity expected from the C4/C4 groups; Ecotox chemical class: surfactant-cationic-C16-N(C4)(C4)CCO; [redacted]; pH 7; hardness <150.0 mg/L as CaCO3; effective concentrations based on 100% active ingredients and mean measured concentrations; and TOC <2.0 mg/L;
high concern for toxicity
mitigation of toxicity expected in the presence of 10 mg TOC/L but will be reduced 30% from the ethoxylate on the quaternary;
assessment factor = 10.0
concern concentration (CC) = 0.004 mg/L with no mitigation factored into the CC

PART V: SUMMARY OF EXPOSURE/RELEASE

Manu:

[redacted]

Use:

[redacted]

PART VI: FOCUS DECISION AND RATIONALE

DISPOSITION: Drop with non 5(e) SNUR

RATIONALE: P04-0625 was dropped with a non 5(e) SNUR for no releases to water. Potential risks to human health were addressed by adequate warnings and PPE. Although concerns were high, potential risks to the environment were low based on no expected releases to water.

PART VII: CCD DISPOSITION / DD

CCD:

STRUCTURE ACTIVITY TEAM REPORT	ver. 04/98	[redacted]	
Case #:	P-04-0625	**DCN:**	
SAT Date:	6/8/2004	**SAT Chair:**	L. Keifer

Submitter: Champion Technologies

Chemical Name:

1-Hexadecanaminium, N,N-dibutyl-N-(2-hydroxyethyl)-, bromide

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

Structure

[redacted]

RECEIVED
PPT OPC

Molecular Formula:	[redacted]		
Molecular Wt.	[redacted]	**WT%<500:**	**WT%<1000:**
MP:	[redacted]	**BP:** Decompo	**Eq. Wt:**
H2O Sol (g/L):	[redacted]	**V.P.**	[redacted]
Max. Prod. Volume (kg/yr):	[redacted]	**Physical State:**	[redacted]

USE:

[redacted]

Related Case Numbers	Case Role	Related Case Numbers	Case Role
[redacted]			

Focus	**Date:** 6/24/04	**Results:** non 5e SNUR - eco

STRUCTURE ACTIVITY TEAM REPORT [redacted] 06/08/04

CASE NUMBER: **P04-0625**

RELATED CASES: [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	2	3

KEYWORDS: IRR-S,E,L,MM CORR LIVER
LUNGS KIDNEY NEURO
DEVEL SENS-S
AQUATOX

SUMMARY OF ASSESSMENT

FATE: [redacted] Estimations for covalent ion pair [redacted] LogBCF = 1.85(E);
POTW removal(%)= 90 via sorption & [redacted]
Time for complete ultimate aerobic biodeg = wk
PBT Potential: P1B1T2
Sorption to soils/sediments = strong - v.strong
*CEB FATE: Migration to ground water = negl

HEALTH: Absorption poor thru skin with irritation based on submitted test data for an analog, good thru lungs and moderate thru GI based on analogs. Concern for irritation and corrosion to all membranes from high ai products based on analog test data and [redacted]; neurotoxicity from the quaternary; lung toxicity if inhaled due to surfactancy for low ai products; developmental toxicity based on [redacted] (rat developmental toxicity NOEL = 50 mg/kg, delayed ossification at 100 mg/kg); and dermal sensitization from the quaternary nitrogen moiety.

*CEB HEALTH: Moderate concern (Dermal, inhalation)

test data for [redacted] were: rat acute oral LD50 = 600 mg/kg with effects to the lungs, liver, kidney, and GI tract irritation; severe skin irritation with corrosion in rabbits

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	<	0.360 P
daphnid 48-h LC50	<	0.960 P
green algal 96-h EC50	<	0.690 P
fish Chronic Value (ChV)	<	0.040 P
daphnid ChV	<	0.100 P
algal ChV	<	0.070 P

Predictions based on SARs for monoalkyl quaternary surfactants C16 and excess toxicity expected from the C4/C4 groups; Ecotox chemical class: surfactant-cationic-C16-N(C4)(C4)CCO; [redacted]; pH 7; hardness <150.0 mg/L as $CaCO_3$; effective concentrations based on 100% active ingredients and mean measured concentrations; and TOC <2.0 mg/L;
high concern for toxicity
mitigation of toxicity expected in the presence of 10 mg TOC/L but will be reduced 30% from the ethoxylate on the quaternary;
assessment factor = 10.0
concern concentration (CC) = 0.004 mg/L with no mitigation factored into the CC
*CEB ECOTOX: All releases to surface waters with CC = 4 ppb

SAT Co-chair: Leonard Keifer 564-8916

GTOX Report

PMN No.
P-04-0625

CAS No.
[redacted]

Rcvd:
05/28/04

OECD
Incomplet

ID: Rec# 5 : 154

S/A
S

Name of Analog

Reviewer
CAA

		with activation	without activation	Positive Strains
Salmonella Assay:				
Chromosomal Aberration	CHO:			
	CHL:			
	V79:			
E. coli Reverse Mutation:				
Mouse Micronucleus Assay:	Route:			
Rat Hepatocytes Unscheduled DNA Synthesis:				

Other GTOX Results

Comments

ECOTOX:

Fate:

[redacted]

WS/Log P:

[redacted]

NCSAB SAT REPORT [redacted]

PMN: P-04-0625	CAS RN: [redacted]

Chemical Name:

1-Hexadecanaminium, N,N-dibutyl-N-(2-hydroxyethyl)-, bromide

Analogs:

Production Volume:

Structure: [redacted]

Use:

[redacted]

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

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	< 0.360		
Daphnid 48-h	< 0.960		
Algal 96-h	< 0.690		
Fish ChV	< 0.036		
Daphnid ChV	< 0.096		
Algal ChV	< 0.069		
BCF			

CHEMICAL CLASS:			SAR: surf - cat - mono - C16	
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION 0.004
DATE 6/8/04			ASSESSOR:	

Environmental Effects Branch

Estimated Toxicity Values for Quaternary Ammonium Surfactants

Assessor	0	Date	06/07/2004
PMN Number	P-04-0625		
Chemical Name	0.00		
Chemical Class	0.00		
Log Kow (CLOGP)	[redacted]		
Log Kow Measured	0.00		
Molecular Weight	[redacted]		
Physical State	[redacted]		
Melting Point	[redacted]		

Measured Water Solubility [redacted]
Estimated Water Solubility, Banerjee equation

QSAR	Toxicity mg/L
Fish Acute LC50, Freshwater -No. Of Carbons, 10-16	0.363
Daphnid Acute LC50 - No. Of Carbons, 10-16	0.959
Snail Acute LC50 - No. of Carbons, 10-16	0.692
Fish Acute LC50, Freshwater - No. of Carbons, 16-2	0.356
Daphnid Acute LC50 - No. of Carbons, 16-22	1.462
Snail Acute LC50 - No. of Carbons, 16-22	0.669

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 6-8-04

ATTENDEES	SIGNATURE
CHEMISTRY	
✓ Paul Bickart	Paul Bickart
Diana Darling	
Rich Engler	
Greg Fritz	
Daniel Lin	
✓ Kathy Schechter	Kathy Schechter
Jenny Tou	
ENVIRONMENTAL FATE	
✓ Bob Boethling	Bob Boethling
Laurence Libelo	
David Lynch	
Andy Mamantov	
Gary Thom	
HEALTH EFFECTS	
Katherine Anitole	
✓ Michael Cimino	Michael C Cimino
Leonard Keifer	
✓ David Lai	David Lai
✓ Jim Murphy	Jim Murphy
Deborah Norris	
✓ Ronald Ward	
Yin Tak Woo	
ENVIRONMENTAL EFFECTS	
✓ Gordon Cash	Gordon Cash
Vince Nabholz	
Campbell, Princes	
SAT CHAIR/OTHER	
Rebecca Jones	
✓ Leonard Keifer	L C Keifer
Vince Nabholz	
✓ Jim Kwiat	J R Kwiat